Laser Spectroscopy of Rare Rubidium Isotopes and Development of Data Analysis Software at TRIUMF

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July 2012

A thesis submitted to McGill University in partial fulfilment of the requirements of the degree of Master of Science

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2012

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Abstract

TRIUMF, Canada's national laboratory for nuclear and particle physics has been peering into the shape and structure of highly unstable, rare isotopes. Employing the method of collinear fast-beam laser spectroscopy, the nuclear ground state spin, hyperfine moments and charge radii can be determined. The laser spectroscopy group at TRIUMF has used this method to investigate the properties of rubidium isotopes, where $^{76-98}$ Rb had been previously studied at ISOLDE by Thibault et al.. Laser spectroscopy was performed at TRIUMF on both the neutron deficient $^{74-76}$ Rb, providing insight into the behaviour leading up to the proton drip line. On the neutron rich end, a programme is in place to extend measurements into the highly deformed ^{98–100}Rb. Preliminary measurements of the spectra of the spin-0 isotope ⁹²Rb have been carried out. on beams with intensities of 10^7s^{-1} , representing the first time heavy rubidiums have been produced and studied spectroscopically at TRIUMF. These measurements have been carried out in conjunction with the implementation of a new MCS based data acquisition system, greatly improving the data collection and analysis capabilities of the laser spectroscopy group.

Résumé

TRIUMF, le laboratoire national canadien pour la recherche en physique nucléaire et en physique des particules, a entrepris l'étude de la forme ainsi que la structure d'isotopes rares et hautement instables. En employant la méthode de la spectroscopie colinéaire utilisant des faisceaux atomiques à haute vitesse, le spin nucléaire ainsi que les moments nucléaires et le rayon de charge peuvent êtres determinés. Le groupe de spectroscopie au laser de TRIUMF a usé de cette méthode pour observer les propriétés fondamentales des isotopes du rubidium, famille isotopique pour laquelle les isotopes ⁷⁶Rb à ⁹⁸Rb ont déjà été étudiés au laboratoire ISOLDE par Thibault *et al.*. En premier lieu, les isotopes déficitaires en neutrons ⁷⁴Rb-⁷⁶Rb ont étés observés, permettant l'étude du rayon de charge nucléaire dans le régime menant à la ligne de limite de stabilité. Du côté riche en neutrons, un programme est en cours pour entreprendre l'étude des isotopes ⁹⁸Rb-¹⁰⁰Rb, ces derniers étant hautement déformés. Des mesures préliminaires sur le spectre hyperfin de l'isotope ⁹²Rb, au spin nucleaire de 0, ont été réalisées, avec un rendement ionique de l'ordre de 10^7 s^{-1} . Ceci représente la première fois que des rubidiums lourds ont été produits et étudiés spectroscopiquement à TRIUMF. Ces nouvelles mesures ont été prises grâce à un nouveau système basé sur le principe d'un MCS, permettant l'augmentation de la capacité ainsi que de la qualité de l'acquisition de données.

Acknowledgements

Under no pretences do I believe this thesis, which is as much a summary of my work as a synthesis of what I have learnt, could have been accomplished by myself alone. I am most indebted to Dr. Fritz Buchinger, for having given me the opportunity to work at TRIUMF and partake in his research, a legacy I shall never forget and will look upon fondly for the rest of my days. I must sincerely thank Prof. John Crawford for his advice, which has proved invaluable time and again as I waded through various unknowns and worked on my data analysis program, for which he must be acknowledged as the inspiration.

I cannot possibly omit thanking Dr. Sid Gulick at McGill, whom I can only conclude has limitless patience, especially after he introduced me to the field, in addition to teaching me how to operate Argon-ion lasers and dye rings.

On the West coast, I am most proud of having been able to work under Dr. Matt Pearson, whose encyclopedic knowledge of all things saved me from headaches time and again. Many thanks to Dr. Ernesto Mané; the long discussions we had about the data analysis programme were crucial to my learning C++ in the first place (the countless laughs also helped). A special thanks to (soon to be Dr.) Annika Voss for walking me around the apparatus, informing me of what not to touch and for moral support as officemate. To Bradley in Manchester: we've had some good laughs (in addition to performing serious scientific measurements)!

Also, I thank the following people at McGill: Phil Lagogiannis, Joel Beaudry, Rob Keyes and Dan Trojand. We should get a coffee sometime.

Last but not least I must thank the most important people in my life: Fanny, for having supported me throughout this journey (I knew you'd love Vancouver). Dad, for having walked me to the science museum in Ottawa as a kid enough times to make me end up at TRIUMF, and Mom, for having encouraged me to make it this far.

I wish you all the very best!

À la mémoire de Sayed

1 A Brief Introduction to Collinear Laser Spectroscopy

1.1 Ground State Nuclear Properties

1.1.1 Physical Properties

The combination of both Electromagnetic and Strong forces will generate what is known as a nuclear potential. When nucleons are confined near each other, they will interact through both these means. The form of the potential, uniquely defined by both the quantity and energies of constituents in the core, determines the overall characteristics of the atomic nucleus. Thus, an immediately relevant characteristic for any nucleus is its mass (m_N) , equal to the rest mass of all constituents minus the overall binding energy:

$$m_N = \sum_{i}^{n} m_i - \frac{E_b}{c^2},$$
 (1.1)

where m_i is the mass of the i^{th} constituent and E_b is the binding energy, also known as the mass defect. With the progress of nuclear science, particularly the technological progression of isotope research¹ facilities worldwide, mappings of nuclear masses have come to span much of the nuclear chart. The nucleus' size is also an extremely useful ground state property: not only does it allow for first order estimates of nuclear density, but its use across chains of isotopes allows one to study the dynamic progression of the overall nuclear configuration. As one modifies the nuclear potential by the addition of neutrons, slight changes in the shape nuclear arrangement will take place.

¹These facilities are often referred to as on line isotope separator facilities (ISOL) due to their primary function: the production and mass separation of unstable isotopes.

Studying the size of the core allows for the identification of deformation, particularly when sudden shifts in size occur from one isotope to the next.

Of course, imaging is out of the question for objects whose diameter is on the order of a few femtometres. Instead, the charge radius is used, defined as the radius over which the electrostatic charge of the protons has a nontrivial effect. In addition, given the possibility for nuclear rotation or vibration, the charge radius is taken as a root-mean-square (RMS) from the set n of observed atoms:

$$\langle r \rangle = \sqrt{\frac{1}{n} \sum_{i}^{n} r_{i}^{2}} \tag{1.2}$$

In the field of nuclear shape and structure, the mean-square charge radius (MSCR), synonymous for RMS charge radius, is a commonly reported value.

1.1.2 Nuclear Moments

The use of nuclear moments also provides clues as to the shape and structure at hand. Given the nonzero spin of both types of nucleons, both carry a quantized, intrinsic magnetic dipole moment $\vec{\mu}_b$. Bearing in mind that spin-up spin-down pairings result in the overall cancellation of the dipole moments within pairs, measuring the overall nuclear magnetic dipole moment $\vec{\mu}_N$ will necessarily yield indirect information on the overall pairings. Furthermore, given the range of theoretical nuclear pairing and structure models currently used in research, the use of the magnetic dipole moment serves as an ideal test for model predictions.

Finally, just as in the classical electrostatic case, the nuclear charge distribution ρ_n , in the case of full sphericity, will have a null electric quadrupole moment Q_2 . Therefore, measuring any nonzero electric quadrupole for a nuclear charge

distribution implies a lack of sphericity, which paves the way for the study of nuclear deformation, an extremely active field of research in nuclear science today. All that is now needed is a method to extract these physical properties and moments from samples of nuclei.

1.2 Laser Spectroscopy

The electronic orbitals which enshroud the nucleus are dependent upon nuclear electrostatic properties. The study of electronic energy levels therefore probes the nucleus itself. Using proper theoretical means, discussed later, one may tie the exact value of electronic levels to properties of the core.

Here, atomic spectroscopy of high precision is needed, requiring a stable, controllable light source - ideally a laser. Properly stabilised lasers can produce light which is monochromatic down to a few MHz. Considering that frequency in the visible spectrum is on the order of several hundred THz, this means modern stabilised lasers have an output stability down to about one part in one hundred million.

Laser spectroscopy works by measuring the hyperfine splitting of spectral lines, a set of Hamiltonian perturbations caused by the interaction between the nuclear magnetic moment (μ_N) and the magnetic field (B_e) of the orbiting electrons, in addition to the presence of an electrostatic quadrupole (Q_2) moment in the nucleus:

$$\Delta E_{HFS} \propto \vec{\mu}_N \cdot \vec{B}_e + eQ_2. \tag{1.3}$$

Obtaining information on this energy splitting naturally produces information on these quantities. If one happens to have access to more than one isotope, it is even possible to infer the relative change in size between the two, by measuring the overall shift in hyperfine line centroid. The former, known as the isotope shift, exists because of the change in nuclear mass and field, due to the introduction of extra neutrons, which acts to slightly perturb each electron's energy level.

This is a particularly tantalising set of circumstances; by merely measuring the splittings and energies of hyperfine multiplets within a spectral line, one can extract information about nuclear moments within the core, in addition to information regarding its size. This is the domain of laser spectroscopy, a powerful tool which provides access to the inner workings of nuclei.

1.3 Collinear Fast-Beam Spectroscopy

In the case where studied isotopes are abundant and sufficiently stable, laser spectroscopy can be performed at room temperature, for example using a vapour cell to contain the sample. However, stable isotopes having been studied long ago, the focus in recent decades has moved onto increasingly unstable and therefore rare isotopes. Amassing sufficient numbers to fill a room-temperature vapour cell is usually not feasible.

The advent of isotope separator facilities such as ISOLDE, ISAC, JYFLTRAP and others has made accessible increasingly unstable and short lived isotopes. Such facilities, which generally produce rare isotopes by proton bombardment of targets, have output energies usually in the tens of keV range. Given both the high energy and short lifetime (usually down to a few milliseconds), the idea of trapping isotopes and confining them to a vessel for study becomes impractical.

These operational constraints have resulted in the birth of collinear fast-beam

spectroscopy. Instead of attempting to hold the isotopes in a sample container, spectroscopy is performed within the high vacuum beamline itself, as the isotopes fly by at high velocity (fast-beam). What is commonly done is to have the laser beam and isotope trajectory overlap in a collinear fashion over a straight beamline segment.

As the isotopes' flight path takes them through the laser beam, which is tuned at their hyperfine resonance, photons are emitted. These are then collected by photomultiplier tubes (PMT's) placed on the outer surfaces of the beamline, and recorded to computer.

This technique provides a unique advantage: high ion velocity results in a decrease of the relative energy spread due to the thermal motion of the particles. Since most isotope separators operate ion beams in the non-relativistic regimes (\sim 30 keV), purely classical energy considerations suffice. Thus, if one considers the kinetic energy as being the total energy of each particle:

$$E = \frac{1}{2}mv^2, \tag{1.4}$$

during delivery, the isotopes possess an energy spread δE , which depends on specifications. This principally thermal spread results in a distribution of velocities δv which, by equation (1.4) is related to δE by:

$$\delta v = \frac{\delta E}{mv}.\tag{1.5}$$

This quantity is fixed: once the isotopes are produced by bombardment of the target (nuclear spallation), they no longer have any means by which to dissipate energy in the vacuum. One can nevertheless minimize δv by increas-



Figure 1: Representation of the kinetic energy of nuclei and of the inverse proportionality between velocity spread δV (expressed as $\beta = \frac{v}{c}$) and velocity. Note that δE , the energy spread is fixed at the time of isotope production and cannot be changed on line.

ing the velocity of the beam, present in the denominator of equation (1.5), by using acceleration electrodes. The net effect of this technique is to narrow the width of the measured spectral lines. This is often referred to as *Doppler free spectroscopy*. The relation between energy and velocity spreads in shown in Figure 1.

Thus, work at isotope separators not only provides access to rare isotopes, it also provides a built-in means to increase the precision of spectroscopic measurements.

1.4 Previous Work

Facilities such as ISOLDE (CERN), LISOL (Leuven), JYFLTRAP (Jyväskylä), in addition to TRIUMF are currently involved in the investigation of rare isotope hyperfine spectra of radioactive isotopes which lie far away from the region of stability. It is in this regime that one encounters exotic particles, with more highly deformed nuclei.

Not only do these isotopes pose a technical challenge, chiefly due to their short lifetime and radiation, they also pose a theoretical one: currently, no single model can accurately predict the wide spectrum of deformations, rotations, vibrations and metastable isomeric states encountered across the nuclear chart. Instead, specific models tend to have their own region of validity, and require increasing amounts of fine-tuning as one departs this domain.

The lack of empirical knowledge regarding these isotopes represents a serious hindrance to the advancement of theoretical descriptions of the atomic nucleus. Certainly, knowing more about ground state properties represents the first step towards constructing a more complete theory governing the nuclear chart.

As an example of the disparity in coverage between stable and unstable isotopes, one may consider Figure 2. Only coloured isotopes have been optically observed by techniques including laser spectroscopy. Isotopes in red were measured prior to 1995, while those in blue occurred after. One observes several gaps in coverage, symptomatic of the difficulties associated with the production of usable quantities of exotic isotopes, often with half-lives in submillisecond range.

As a gauge to the technical nature of the challenge, it is worth noting that for highly unstable isotopes (either neutron rich or deficient), it is not uncommon



Figure 2: The nuclear chart representing all known elements and their isotopes. Isotopes coloured red have been optically measured prior to 1995, while blue ones were observed after. Obtained from [1].

to encounter isotope separator yields on the order of 10^3 ions/s. Extending coverage into high instability zones in past years has thus been directly equivalent to developing strategies to counter these extremely small yields.

1.5 This Work

This M.Sc. thesis presents the focus of the author's work and studies while stationed at TRIUMF, working with the collinear fast-beam spectroscopy (CFBS) group, itself a collaboration between TRIUMF, the University of Manchester and McGill.

In particular, the work done in this thesis has had as a central theme the study of both neutron-deficient and neutron-rich rubidium. The element has been under intense scrutiny at TRIUMF in the past two years, chiefly because of the high degree of deformation known to exist as one strays away from the stable isotopes 85 Rb & 87 Rb.

The thesis is presented in two separate sections, one focusing on the practical relationships used in collinear spectroscopy to extract ground state moments and nuclear spins, in addition to an overview of the current body of knowledge on rubidium ground state moments. In this same section, recent CFBS results are presented and discussed. Particular emphasis is placed on ⁹²Rb, which is to be used in the future by the group as a frequency standard.

The second half is entirely devoted to the development of a new data analysis program, HInSane, whose stated goal is to perform the relevant analyses on hyperfine (HF) spectra, allowing the extraction of hyperfine coefficients, etc.. The author of this thesis participated with the CFBS group in the experimental run setup and data acquisition of rare isotope HF spectra, including the rubidiums presented herein. As for the data analysis program, itself an extensive modification of a pre-existing TRIUMF data format conversion routine, the author was solely responsible for implementing the main features discussed within this work. The hyperfine spectrum simulation was originally written in MATLAB by Prof. John Crawford (McGill), and required extensive modification by the author to port the routine to C++. Certainly, this work was only possible after extensive discussion with other CFBS group members.

2 The Hyperfine Structure and Spectroscopic Observables

2.1 The Fine and Hyperfine Structure of Spectral Lines

Electrons exist in discrete energy levels within an atom. Electronic de-excitation results in the emission of light at discrete wavelengths corresponding to the energy difference between ground and excited states. As the scheme of possible energy levels depends on the nuclear potential and electronic configurations, each element has its unique set of discrete spectral lines.

Early investigations of electronic spectra used elemental gas discharge lamps to record several narrow lines of light across the visible spectrum. These lines would prove essential for the early understanding of the atom-electron system. Unbeknown to early experimentalists, *a priori* discrete lines were in reality a complicated collection of closely spaced, extremely narrow emission wavelengths, which group together in tight clusters, all of these working within the coarse electronic emission line itself. The eventual discovery of these minuscule constituents was very much in tune with the advancement of spectroscopic techniques and the refinement of available equipment.

The splittings were first discovered and dubbed the *fine structure* of spectral lines, due to both quantum and relativistic Hamiltonian corrections. It was later discovered by Michelson in 1881 that the fine structure splittings decomposed into still smaller lines, when resolved with sufficient precision. These were dubbed the hyperfine structure (HFS). To this day, the HFS remains the finest possibly *observable* feature in the spectra of atoms. As an example, the sequence from coarse to hyperfine lines in sodium is shown in Figure 3.



Figure 3: The sodium D lines, shown in progressively higher resolution. To the left, the coarse spectral line is visible, in the form of a single electronic transition. After first order Hamiltonian corrections, the fine structure becomes apparent in the middle, while to the right one may observe the hyperfine structure, after taking into account nuclear properties. The Bohr line refers to what would be visible at low resolution - an apparent singlet. Note that level splittings are not to scale. The fine structure is generally on the order of milielectronvolts (meV), while the hyperfine splitting is on the order of microelectronvolts (μ eV). The quantum number F=I+J represents the sum of nuclear and electronic angular momentum.

There initially existed no theoretical grounding to explain the mechanism by which spectral lines decomposed into these constituents. One would have to await the advancement of quantum mechanics and the birth of special relativity to make sense of the hitherto unexpected development. It followed that the fine structure, itself both an energy shift added to the old quantum prediction, and a splitting of the line itself, was attributable to a relativistic kinetic energy substitution producing a shift on the order of 10^{-5} eV:

$$K = \frac{p^2}{2m} \to \sqrt{p^2 c^2 - m^2 c^4} - mc^2$$
 (2.1)

The line splitting itself follows from the coupling of two angular momentum electronic quantum numbers, L (orbital) and S $(\text{spin})^2$, in the form of a dot product of both vectors

$$\Delta E_{FS} \propto \vec{L} \cdot \vec{S}. \tag{2.2}$$

Given that the electron spin may be up or down this results in two distinct possibilities for ΔE_{FS} , resulting in two fine structure sub-lines.

The hyperfine structure, on the other hand, arises from the fact that both the atomic nucleus and the electrons around it are electrically charged entities which are always in motion. On the one hand, it is due to the interaction between the nuclear magnetic dipole $(\vec{\mu}_I)$ of the core, resulting from the total angular momentum of the nucleus (I) and of the magnetic field (\vec{B}_e) of the electron distribution in and around the atomic nucleus. Mathematically, $\vec{\mu}_I$ may possess values defined by

$$\vec{\mu}_I = g_I \frac{2}{2m_p} \vec{I},\tag{2.3}$$

²This is known as Russell-Saunders coupling.

where g_I is the nuclear gyromagnetic ratio and m_p is the proton mass. As with many quantities derived from quantum mechanics, the vector $\vec{\mu}_I$ is quantized, restricted to half-integer multiples of I.

On the other hand, the field \vec{B}_e arises from the collective motion of the electrons. This can then be deconstructed into two linearly independent forms, corresponding to the electronic spin (s), and the orbital angular momentum (1):

$$\vec{B} = \vec{B}_s + \vec{B}_l. \tag{2.4}$$

The exact form of the electronic magnetic field contributions are more complicated, due to the necessity of applying the Biot-Savart law [2] to extract the field from the electron current generated by their orbital and spin motions:

$$\vec{B}_s = \frac{\mu_0}{4\pi r^3} (3(\vec{\mu}_s^e \cdot \hat{r})\hat{r} - \vec{\mu}_s^e) + \frac{2\mu_0}{3}\delta^3(r)\vec{\mu}_s^e, \qquad (2.5)$$

$$\vec{B}_l = -2\mu_B \frac{\mu_0}{4\pi r^3} \vec{l}.$$
 (2.6)

Here, μ_0 is the vacuum permeability constant, μ_B is the Bohr Magneton, μ_s^e is the intrinsic electron magnetic moment, r is the distance from coordinate centre (nuclear core) to the electron's position and $\delta^3(r)$ is the three dimensional Dirac delta function, arising from the fact that the electrons are considered to be perfect point sources. In equation (2.6), the vector \vec{l} is the orbital angular momentum vector of the electrons.

In addition, the electric contribution to the hyperfine structure originates from the presence of a nonzero electric quadrupole, Q_2 , which will act to perturb the shift caused by the magnetic interaction. It is worthwhile noting that this effect is generally much smaller than the magnetic contribution which, to first approximation, may be considered to generate the overall hyperfine splitting, generally by about two orders of magnitude. More details regarding electric quadrupoles will be presented in the next section.

The interaction between the nuclear magnetic moment and electronic magnetic field is then simply expressed as the dot product between both resulting vectors, while the electrostatic contribution consists of the quadrupole multiplied by the electric field gradient:

$$H_{HF} = -\vec{\mu}_I \cdot \vec{B}_e + eQ_2 \frac{\partial^2 V}{\partial z^2}.$$
(2.7)

Strictly speaking, H_{HF} represents the energy imparted (or taken from) the electrons due to the electromagnetic interaction between themselves and the nucleus. The interaction results in a slight perturbation of the energy scheme of the electrons from their orbital energies.

Thus, to first approximation, to obtain the energy of each possible hyperfine line, one must run the quantum numbers L,S and I in equations (2.3), (2.5) & (2.6), then apply equation (2.7).

This produces all possible angular momentum pairing combinations. For each of these, there will be one resulting energy perturbation, producing a hyperfine line.

In other words, the centroid (middle) of the coarse spectral lines corresponds to the average energy given away by de-exciting electrons. As the HFS chiefly depends on the atomic nucleus, measuring it allows one to access information about the nuclear core.

2.2 Excited States, Deformation and Quadrupoles

Instability may be quantified by examining the binding energy per nucleon. Strictly speaking, this quantity measures the amount of energy which must be supplied to remove a nucleon from the core. Einstein's most famous equation dictates that:

$$E = mc^2 \tag{2.8}$$

Therefore, the overall binding energy stored in a nucleon measures how strongly each constituent is *trapped* inside the nuclear potential well, manifest as a reduction in the mass of the nucleus vis-a-vis that of the unpaired nucleons alone, as shown in equation 1.1.

As the nuclei increase in number of constituents, thereby increasing the net positive charge of the core, the Coulomb repulsion between the protons becomes a significant destabilising agent, making it easier for nucleons to escape by reducing the overall binding energy: first, it may render the nucleus unstable, making it susceptible to radioactive decay. Second, it is possible that the shape of the nucleus deviates from a spherically symmetric one, to more exotic shapes. This phenomenon exists to varying degrees in the heavy elements with Z > 82 and $150 \leq A \leq 180$, as well as $A \gtrsim 250$ [3].

There also exists a wide spectrum of possible arrangements for a given quantity of nucleons within the core. These are known as isomeric states or simply, isomers, and occur when a nucleon finds itself in an excited orbital state. Such nuclei will possess different intrinsic properties, depending on the nucleon configuration. Thus nuclear spin (I), magnetic dipole moment (μ_B), parity (π), charge conjugation (C) and of course, binding energy (E_b) are likely to differ from one isomer to the next. Isomers are denoted by using a lowercase m^3 by the atomic mass, all in superscript. For example, 98m Rb denotes a metastable isomer of 98 Rb. Isomeric decays always involve the release of a gamma ray photon:

$${}^{Am}X \to {}^{A}X + \gamma, \tag{2.9}$$

where the photon's energy corresponds to the energy of the excited nucleon, which returns to its ground state nuclear orbital.

Intimately linked to stability is the shape of the core itself. An isotropic nuclear core will, via the symmetry of the spherical arrangement, offer the highest degree of binding between nucleons. It is thus unsurprising to find that unstable atoms generally come equipped with deformed cores, while magic number⁴ nuclei are generally spherical. It is then relevant to briefly consider the possible shapes an unstable atomic nucleus may take, as well as the physical consequences of such a deformation.

First order deformations may be obtained by considering single-axis spherical deformations, as shown in Figure 4. This phenomena exists to varying degrees in the heavy, unstable elements. The examples of prolate and oblate spheroids also provides insight into how one may proceed to determine the overall deformation.

Considering the electric potential V of a sphere with charge e and radius r, evaluated at a distance D, nuclear deformation may be measured by observing

³m stands for metastable.

 $^{^4\}mathrm{Magic}$ numbers refer to nuclear shell closures predicted by the shell model. These correspond to 2,8,20,28,50,82,126,..



Figure 4: Representation of the possible first order deformation modes of a sphere. Left: an oblate spheroid, whose polar radius is shorter than the equatorial one. Right: a prolate spheroid, whose polar radius exceeds the equatorial one.

the behaviour of the first three terms of the potential's series expansion [4]:

$$V = \frac{e}{D} + \frac{er}{D^2}\cos\theta + \frac{er^2}{D^3}\left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right) + \dots$$
(2.10)

In the case of a *perfect* charged sphere the only nonzero moment is the monopole, equal to the overall charge. This corresponds to the first term in equation (2.10).

Taking the gradient of V to obtain the electric field will always eliminate the $\frac{1}{D^2}$ contribution. What remains is the quadrupole term of order $\frac{1}{D^3}$, which is only zero in absence of deformation.

Specifically, electric n-poles from the multipole expansion of a sphere are used to quantify deformation [5]:

$$Q_l = \int d^3 r r^l P_l(\cos\theta)\rho(r) \tag{2.11}$$

where $P_l(\cos\theta)$ is the Legendre polynomial of degree l and $\rho(r)$ is the charge distribution within the nucleus. In this case, the electric quadrupole moment corresponds to the l = 2 case:

$$Q_2 = \int d^3 r (3z^2 - r^2) \rho(r). \qquad (2.12)$$

In equation (2.12), z represents the axis of elongation. Just as the potential V of equation (2.10), the quadrupole moment will be nonzero only if deformation is present. Unfortunately, common practice is to label the quadrupole moment Q_0 , which at first sight may be confused for the monopole term. The former labelling is intended to reflect the classical nature of the observable.

Regardless of convention, this quantity is absolutely crucial to the study of nuclei, permitting the quantitative analysis of shape deformation.

A common parametrisation for the deformation of a sphere uses a shape function defined in terms of spherical harmonics. As the series is infinite, the mathematics rapidly increase in complexity and scope. Fortunately, quantities of relevance to extracting Q_2 may be considered by using the first few terms only.

Assuming the spherical deformation mode is volume conserving [3], the shape of the charge distribution may be represented by the parametrisation:

$$R(\theta) = R_0 \left[1 + \sum_{n=2}^n \left(\beta_n Y_{n0}(\theta, 0) - \frac{\beta_n^2}{4\pi} \right) \right].$$
 (2.13)

With the spherical harmonics taken to be symmetric in cylindrical coordinates, eliminating the ϕ dependency. equation (2.13) is linked to the multipole expansion via:

$$Q_l = \frac{3}{8\pi} M R(\theta), \qquad (2.14)$$

where M is the mass of the nucleus. Assuming equation (2.13) represents the

charge distribution, it follows that the electric quadrupole moment, expressed in terms of the β_n expansion coefficients, with the Y_{lm} numerically evaluated, may be written as [1]:

$$Q_0 \approx \frac{5Zr_{sph}^2}{\sqrt{5\pi}} \langle \beta_2 \rangle (1 + 0.36 \langle \beta_2 \rangle), \qquad (2.15)$$

where the expansion is only carried out for n = 2, higher order terms being of vanishing contribution. Note that the radius is denoted r_{sph} , being the radius of the original sphere, which is deformed by nonzero values of $\langle \beta_2 \rangle$. For $\langle \beta_2 \rangle$ ≈ 0 , Q_0 vanishes. Positive values of $\langle \beta_2 \rangle$ indicate prolate deformation, while negative ones arise for oblate.

2.3 Spectroscopic Observables

Theoretically, the spacing of each hyperfine peak relative to the unperturbed centroid energy⁵ is given by [6]:

$$\Delta E = \frac{K}{2}A - \frac{3K(K+1) - 4I(I+1)J(J+1)}{8I(2I-1)J(2J-1)}B,$$
(2.16)

where

$$K = F(F+1) - I(I+1) - J(J+1)$$
(2.17)

and A,B represent the hyperfine coefficients:

$$A = \frac{\mu_I}{IJ} B_e(0), \qquad (2.18)$$

⁵This overall centroid energy corresponds to the weighted average of the HF peak energy and their respective amplitudes. As an example, considering a set of hyperfine lines of different amplitudes, the weighted average of their energies & intensities would correspond to the perceived energy of the spectral line, should the HFS not be resolved.

$$B = eQ_S \left\langle \frac{\partial^2 V}{\partial z^2} \right\rangle. \tag{2.19}$$

Note that equation 2.16 is analogous to equation 2.7. Inspection of the terms in equations (2.18) and (2.19) reveal what they encode: The A coefficient carries information relevant to the magnetic moment of the nuclear core, as well as the overall electronic magnetic field B_e , evaluated at the centre of the nuclear charge distribution. The B coefficient contains information relevant to the electric field gradient. Equation (2.16) thus prescribes a series of splittings from the centroid energy, one per value of (I,J,F), which defines the location of the hyperfine peak centroids.

In general, the A coefficient will outweigh B in terms of magnitude, sometimes by a factor of up to 100. The relative contributions of both A and B are shown in Figure 5, for the case of the spin-4 isomer 78m Rb.

Unfortunately, given both the possible anisotropy of nuclear shape and the possibility of centre-of-mass motion of the nucleus, measurements of the nuclear radius are not commonly reported values. Instead, the mean square charge radius, often cited as the RMS charge radius shown in equation 1.2, is used. This can, to first approximation, be thought of as the radius of the nucleus⁶. It is defined as [7]:

$$\langle r^2 \rangle \approx \frac{3}{5} (r_0 A^{\frac{1}{3}})^2 \left(1 + \frac{5}{4\pi} \langle \beta^2 \rangle \right), \qquad (2.20)$$

where A is the atomic number and $r_0 = 1.2$ fm. Using the RMS charge radius, $\langle r \rangle^2$ allows for the comparative study of nuclear radii across isotopic chains. The onset of nuclear deformation may then be evidenced by systematic changes

 $^{^{6}}$ The quantum mechanical nature of constituent nucleons implies the nucleus has no *hard* surface, but rather a diffuse boundary, where the nuclear wavefunction falls to zero amplitude



Figure 5: Relative contribution of A & B coefficients to hyperfine splitting in 78m Rb. Note that the overall frequency shift of the hyperfine structure (in MHz) is displayed to the left of each level, relative to the unperturbed level (dotted line).

in the MSCR, greater than what would be expected in the case of a perfect spherical $\rho(\mathbf{r})$. Furthermore, variations in the MSCR may be extracted from spectroscopic measurements with relative ease, by measuring isotope shifts.

2.4 Hyperfine Lines

With equation (2.16) detailing the position of hyperfine lines in atoms, one may now discuss their shape. In principle, as the atomic line is discrete, corresponding to the splitting between two electronic levels, *a priori*, one would expect discrete values with no spread.

This is, however, not the case: Each hyperfine spectral line will possess a finite

energy spread which can be simply explained by the Uncertainty Principle:

$$\Delta E \gtrsim \frac{\hbar}{\Delta t} \tag{2.21}$$

Energy spread being linked to the reciprocal of time uncertainty, the spectral line will possess a natural width corresponding to the natural decay time of the hyperfine level. While this effect is extremely small it is, nevertheless, nonzero. The listed lifetime τ of elements of the ⁸⁷Rb hyperfine structure is of ~ 26.3 ns, corresponding to natural linewidth of 6 MHz.

In addition, thermal energy contained in an atomic sample, generating a Boltzmann like thermal distribution, will result in Doppler broadening of the spectral line. This can be understood by considering the isotropic nature of the distribution: The higher the temperature (energy) of the sample, the higher the Doppler shift of constituents with nonzero velocity vectors along the observation axis. Particles with a net nonzero velocity moving towards (or away) from the laser will have slightly shifted hyperfine centroids, resulting in a wider spectral line. This serves as a reminder of the motivation to cool atomic samples as much as possible during spectroscopic measurements - the associated reduction in energy spread.

Practically, the shape of a given hyperfine line is described using the Voigt profile, which is defined as a Doppler broadened Lorentzian distribution. Mathematically one may express the Voigt profile, as a function of frequency ν as:

$$V(\nu) = rl(\nu) + (1 - r)g(\nu)$$
(2.22)

 $r \in [0,1],$



Comparison of Gaussian, Lorentzian and Voigt profiles

Figure 6: Comparison of Gaussian (red), Lorentzian (blue) and Voigt (green) profiles.

where $g(\nu)$ denotes a standard Gaussian function and $l(\nu)$ denotes the Lorentzian contribution:

$$g(\nu) = A_0 exp\left(\frac{-(\nu-\mu)^2}{2\sigma^2}\right)$$
(2.23)

$$l(\nu) = A_0 exp\left(\frac{1}{1 + \frac{2(\nu - \nu_0)^2}{\sigma_\nu}}\right)$$
(2.24)

In both equations (2.23) and (2.24), A_0 is the height parameter, μ is the mean, σ the linewidth (standard deviation). Both functions comprising equation (2.22) are scaled via the weighting factor r, which determines the degree of Doppler broadening [8]. Each of equations (2.22) (2.23) and (2.24) is shown in Figure 6.

Electrostatic acceleration of the ion bunch, travelling collinear to the laser, emitting at frequency ν_{laser} , introduces another Doppler shift to the hyperfine line. Unlike thermal effects, this shift will not influence the linewidth, rather it



Magnitude of Electrostatic Doppler Shift vs. Beam Energy

Figure 7: Representation of equation (2.25), showing the magnitude of electrostatically induced Doppler shift on the hyperfine centroid of an ion bunch. Note that for small energy variation, on the order of a dozen eV, the relation may be taken as approximately linear.

will introduce a multiplicative shift which is exploited to bring the ion bunch into resonance with the laser, by accelerating it to the appropriate velocity. For a centroid of frequency ν , originating from an ion bunch travelling at $\beta = \frac{v}{c}$, this Doppler shift may be expressed as:

$$\nu = \nu_{laser} \sqrt{\frac{1+\beta}{1-\beta}}.$$
(2.25)

The relativistic β parameter is defined as:

$$\beta = \sqrt{2 \frac{E_{bunch}}{E_{mass}}} \tag{2.26}$$

where the numerator is the total kinetic energy of the ion bunch and the

denominator is the rest mass is expressed in terms of equation (2.8). A plot of equation (2.25) is shown in Figure 7.

PMT statistics associated with photon observations will be that of Poisson count statistics. This implies that the uncertainty associated with PMT counts C will be:

$$\delta C = \sqrt{C} \tag{2.27}$$

Hence the uncertainties associated with each point representing a hyperfine line will be the square root of its height, which will be the guiding assumption throughout this work for error analysis.

2.5 Isotope Shifts

Probing the behaviour of the MSCR (equation 2.20) along an isotope chain, the variation in hyperfine centroid energy is measured. This is known as the isotope shift, and provides another strong indicator of the behaviour of nuclear shape. Moving up along a chain, the shape and amplitude of the overall charge distribution slightly changes. Consequently, spectral lines at a photon frequency ν for one isotope will be displaced, and have a value ν ' for the next. The centroid shift between two isotopes A and A' may itself be decomposed into two separate contributions:

$$\delta\nu^{AA'} = \delta\nu^{AA'}_{MS} + \delta\nu^{AA'}_{FS}, \qquad (2.28)$$

with the terms being the mass shift and field shift, respectively. The mass shift is a kinematic effect, which is due to the difference in nuclear mass attributable to differing neutron numbers. The mass shift decomposes into two separate
contributions: the normal mass shift (NMS, or Bohr shift) and the specific mass shift (SMS). The normal mass shift may be expressed as:

$$\delta\nu_{NMS}^{AA'} = \frac{\nu}{1836} \left(\frac{A'-A}{AA'}\right). \tag{2.29}$$

With ν being the transition frequency [9]. The SMS is due to inter-electronic correlations and is incalculable for Z > 2 [9]. Nevertheless, the SMS does display the same reduced mass dependency as does the NMS and may be inferred from measurements of adjacent isotope chains, in an empirical manner. On the other hand, the field shift⁷, due to the perturbation of the electronic orbitals by the modification in shape of the nuclear potential, may be expressed as [1]:

$$\delta\nu_{FS}^{AA'} = \frac{\pi a_0^3}{Z} \beta_s \Delta |\psi(0)|^2 f(Z) \delta \langle r^2 \rangle^{AA'}.$$
(2.30)

 a_0 is the Bohr radius, Z is the atomic number, β_s is an electron screening factor [7] and f(Z) is a relativistic correction. Use of equation (2.30) requires knowledge of $\Delta |\psi(0)|^2$, the change in electron wavefunction evaluated at the core of the nucleus, in addition to f(Z). Both factors must be extracted from model calculations or, in some cases, may be obtained from other isotope shift measurements [6]. Further, equation (2.30) only describes changes in the MSCR, not absolute values. Since the shape of electron orbitals is both highly complex and generally of zero amplitude at the core, equation (2.30) justifies the study of transitions involving S and P orbitals, both isotropic and nonzero⁸ at $\psi(0)$. The D₂ electronic emission line is generally studied, with a $S_{\frac{1}{2}} \rightarrow P_{\frac{3}{2}}$ transition effectively providing information about the core.

⁷The field shift is also known as the volume shift.

 $^{^{8}\}mathrm{Which}$ means that the electron effectively spends some of its time inside the atomic nucleus itself

2.6 Changes in Mean Square Charge Radius

In any isotope chain, some degree of variation is to be expected in the physical properties between members. As supplemental nucleons are added to the nuclear well, occupying higher and higher orbitals, the overall shape of the arrangement can therefore be expected to vary.

While using the MSCR to study shape change does not allow its complete qualification, it is sensitive to the onset of deformation, even in the case where the volume conservation hypothesis in equation (2.15) does not strictly hold. Nevertheless, extracting quadrupole moments from an unpolarised distribution of atoms will effectively yield information about the shape. Thus, deformation will be evidenced by changes in MSCR compared to perfect sphericity [6]. In particular, when data for several adjacent isotopes is available, the presence and evolution of deformation may be evidenced by the rate at which the MSCR changes. Sudden, drastic reversals in trend indicate that the morphology of the nucleus is likely undergoing considerable variation.

The commonly reported variable is not $\langle r^2 \rangle$ but $\delta \langle r^2 \rangle$, the variation in MSCR for an isotope A with regard to a reference isotope:

$$\delta \langle r^2 \rangle = \langle r^2 \rangle^{A'} - \langle r^2 \rangle^{ref}, \qquad (2.31)$$

generally the reference isotope being the most stable (or most easily produced) one. Practically, $\delta \langle r^2 \rangle$ may be extracted by finding the field shift and using equation (2.30). While finding the terms for the previous equation demands detailed theoretical calculations, given the absence of neutron dependant variables, one may then use equation (2.30) consistently across an isotope chain, simply subtracting off the mass shift before extracting $\delta \langle r^2 \rangle$. A common feature for the MSCR along an isotope chain is known as odd-even staggering (OES), corresponding to an alternation in $\delta \langle r^2 \rangle$ between odd-N and even-N nuclei. While theoretical descriptions of OES are model-dependent, the root cause for the phenomenon lies in the fact that nuclei with an odd number of constituents are less tightly bound [10] due to the unpaired nucleon. The pairing correlations between an even number of like nucleons thus works to increase the overall binding in the nuclear potential.

Satula *et al.* have demonstrated [10] that OES in light and medium nuclei are not only due to pairing correlation, but also due to mean-field deformation. In other words, the mean potential seen by individual nucleons, discussed for the shell model, loses its spherical symmetry for unpaired nucleons, resulting in the deformation of nuclear orbitals. In MSCR variations, odd-N isotopes generally possess smaller charge radii than their even-N neighbours. This is, however, not a strict rule. Certain isotopic chains display a reversal in OES, with the even-N members possessing a larger MSCR.

Shell closures may be observed in isotope chains via MSCR variations, corresponding to magic numbers of nucleons. It is a typical feature for many elements to display a characteristic kink in $\delta \langle r^2 \rangle$ at N=28,50 and 126, indicating a sudden change in trend on either side of the magic number. On the neutron rich side, it is common for medium-mass nuclei (A ~ 100) to display rapid MSCR increase as one progresses away from the shell closure.

Reproducing both the OES and sudden MSCR increase remains a challenge to nuclear models.

As an example, the krypton isotope chain is shown in Figure 8. The data reveals a prominent shell closure at N = 50. In addition, a small degree of OES is observable throughout the chain. Further inspection allows one



Figure 8: Variation in RMS charge radius for the krypton isotope chain. Maximum errors are on the order of 1%. Consequently, error bars are too small to be seen by the naked eye. Data obtained from [11].

to make qualitative statements regarding the morphology of the Kr isotopes: deformation is present in both the neutron deficient and rich sides of the N = 50 closure, with more drastic deformation present in neutron-rich isotopes.

3 The CFBS Experiment

3.1 The Spectroscopy Beamline at TRIUMF

3.1.1 Facility Overview

The TRIUMF facility, in Vancouver, B.C. is built around a 500 MeV cyclotron, the largest in the world, and is capable of producing twin proton beams with up to $\sim 350\mu$ A at up to 520MeV.

Branching off the main cyclotron beamline are several experimental setups, operated by internationally coordinated academic and industrial collaborations. The activities carried out on location range from studies of supernova nucleosynthesis to various types of radiotherapy treatments for cancers and other diseases.

The ISAC (Isotope Separator and ACcelerator) halls house newer facilities, built in the late 1990's, which are capable of producing a wide array of rare, radioactive isotopes - a feat only a handful of laboratories in the world may boast. This is accomplished by bombarding a thick target of uranium carbide (UCx) or niobium, as used for this work, with the 520 MeV proton beam generated by the cyclotron. The ISAC facility thus presents an ideal location



Figure 9: Picture of the main beamline. The concentric coils may be used to polarise the ion beam.



Figure 10: Schematic representation of the CFBS beamline (right), the RFQ (Radio Frequency Quadrupole, a Paul Trap) and the switchyard (centre), fed by the ISAC DC ion beam. Approximate scale is shown at the bottom.

for spectroscopic investigations of rare isotopes, many of which have yet to be studied due to the difficulties associated with their production and confinement.

Within ISAC-I, laser spectroscopic investigations of ground-state hyperfine spectra permit the identification of fundamental nuclear properties, including the nuclear spin, moments and charge radii of rare isotopes.

The CFBS apparatus is shown in Figure 10, while a detailed closeup of the beamline segment in which measurements are taken is shown in Figure 11.



Figure 11: The CFBS beamline segment. The incoming cooled ion bunch (left) traverses a voltage gradient where it is accelerated into resonance with a counter-propagating laser. The ions then enter a charge exchange cell filled with hot Na vapour, where they are neutralised. Upon exiting the cell, the neutral atoms undergo resonance with the laser, as shown at the bottom. The emitted photons are recorded by the PMT. Note that both charge exchange cell and acceleration electrodes are floated to the same potential.

The beamline segment of Figure 11, in addition to the elements shown in Figure 10, the setup contains several steering electrodes, in addition to ion beam down the line during calibration. The MCPs, which generate an electrical signal upon being struck by ions, are pulled out of the beamline segments via pneumatic linear feedthroughs to allow unobstructed ion flight. Each type of ion requires its own electrostatic tune down the beamline, since the RFQ is mass dependent.

The ISAC beamline feeds both the TITAN and CFBS collaborations, which branch off the former in a triangular switchyard segment, visible in Figure 10, allowing steering of incoming ions either to the upper RFQ or straight through to the CFBS beamline. Inside the latter, the ions are excited by a laser in collinear geometry to the beamline, and the produced photons are detected by a radially mounted PMT.

3.1.2 The RFQ Ion Trap

The technique of spectroscopy on cooled, bunched beams allows reductions in background of two orders of magnitude [6]. The RFQ cooler-buncher ion trap forms one of the critical components of the experiment, itself belonging to the TITAN collaboration. The RFQ consists of a segmented quadrupole ion trap, combining both an RF electric oscillation providing radial ion confinement, and a set of differentially applied DC voltages, which provide axial trapping, as shown in Figure 12.

The goal of the RFQ is to collect as many ions as possible by lowering the front-end DC potential to zero. Once sufficient ions fly inside the RFQ, over the course of a few milliseconds, the entry voltage is raised, trapping the ions.



CROSS-SECTION

Figure 12: RFQ radial electric fields (top) and axial trapping potential (bottom). The red segments in the axial profile represent the segmented quadrupole electrodes, colour coded with DC potential.

An ambient buffer gas of high purity⁹, helium, is maintained at a partial pressure of 10^{-2} Torr. Collisional cooling between the trapped ions and the buffer gas, in addition to energy losses imparted by the linearly increasing potential gradient shown in Figure 12 reduces the energy spread of the ion bunch, resulting in a decrease of the ion velocities, which obeys the relation [12]:

$$v(t) = |\vec{v}_0| exp\left(\frac{|\vec{E}| - qt}{|\vec{v}_0|}\right).$$
(3.1)

Here v_0 is the initial ion velocity in the trap, m is the ion mass, q is the ion charge and the ratio E/v_0 represents the electron mobility (K). Since the ions in the trap lie within an RF oscillating electric field, they will undergo forced oscillatory motion. Thus, equation (3.1) only represents the envelope of the

⁹Common impurities are water vapour and oxygen, which will result in the formation of oxides with the highly reactive ions.

ions velocity function.

Since the spatial position is related to the velocity function by an integral, assuming no time-dependence of the variables in equation (3.1), one may assert that the exponential function remains unchanged, thus:

$$x(t) \propto C_1 e^{-at}$$

$$C_1 = -\frac{1}{a}$$

$$a = \frac{|\vec{E}|}{|\vec{v_0}|} \frac{q}{m}.$$
(3.2)

One finds that as for the velocity, the spatial position of the ions in the RFQ suffers a time dependant exponential decay. As v(t) in equation (3.1), x(t) only reflects the approximate behaviour of the position envelope. The advantage of the RFQ cooling-bunching process is easily understood: By confining the ions to a smaller region of space, packing them tightly, they will be more easy to excite and observe, due to the bunch's higher density. Typical cooling times in the RFQ range from 1 to 100 ms.

The previous analysis does not take into account other, more subtle effects such as RF heating and inter-ion space-charge repulsion, both factors which will work against the tendency of the bunch to decrease in volume. The latter should remain minimal, so long as particle yields remain in the vicinity of 10^4 to 10^5 ions/bunch [13].

With the bunch cooled and confined to a smaller volume, the ions are ejected by lowering the entrance DC voltage and raising the rear DC voltage. Another advantage becomes apparent: by confining the ions to a bunch of known energy, it is possible to deduce the time at which they will reach the PMT's aperture. By only collecting photons at that time, further background reduction, on the order of 4 orders of magnitude, is achieved.

3.1.3 Vapour Cell Neutralisation

Spectroscopy on Rb is carried out on neutral atoms. The ions are neutralised in a Na vapour cell. The bunch flies down the beamline, shown in Figure 11, collinear to a laser beam which is held slightly off-resonance. The PMT is located in what is known as the interaction region, which contains acceleration electrodes and the charge exchange cell which electrically neutralises the ions. The cell operates by boiling an alkali vapour across the ions' flight path. When both collide, valence electrons are ripped off the vapour atoms by the ions, which regain their neutrality.

The cell can either be operated with Na or Rb vapour, depending on the electrical properties of the ions. It is necessary to ensure the ionisation energy of the chosen elemental vapour's valence electrons closely matches the kinetic energy of the collisions to ensure proper neutralisation. Typical neutralisation efficiencies typically lie above 0.5, meaning half or more of the incoming ion bunch will be observable with the laser. This turns out to be advantageous: Higher neutralisation would introduce energy broadening to the timebunch. The ions crossing the interaction region are accelerated by a voltage gradient

imposed in front of the vapour cell. After neutralisation, the atoms are immune to the effects of the electrostatic steering elements. If the calibration of both laser and beamline energies has been done correctly, the newly neutralised atoms flying out of the cell should see the laser frequency Doppler shifted into resonance. Thereupon, an immediate electronic excitation-de excitation cycle begins, with photons being isotropically emitted¹⁰ within the interaction region, where a spherical mirror (not shown in Figure 11) is located opposite the atom beam's trajectory from the PMT. The mirror has its focus on the PMT lens and effectively increases the solid-angle coverage of the latter, resulting in greater photon counts.

In a typical experiment, the first transmission tunes are accomplished by using stable, abundant isotopes such as 23 Na or 238 U, which require no bunching in the RFQ due to their numbers - on the order of 10^6 ions/s or more. This way, vapour cell performance may be gauged prior to radioactive beam injection. Rare isotope beams, on the other hand, generally require cooling-bunching, as their counts vary from to 10^5 ions/s for stable rubidium down to 10^3 ions/s or less for highly unstable isotopes, such as 98 Rb [14].

3.2 Isotope Shift Measurements

Measuring isotope shifts is not merely a question of recording a single hyperfine peak and comparing to that of another isotope. One must take into account the systematics of the ion beam delivery energy, which is subject to variations on the order of a few volts. Given typical beam energies (20 keV) and an atomic mass on the order of 87 (in the case of rubidium), the voltage to frequencyspace conversion amounts to roughly 6MHz per volt.

Given that isotope shift values typically lie around several hundred MHz, a beam energy drift of no more than two volts introduces a systematic error to measured isotope shifts on the order of one percent.

Typically, what is done to tackle this risk is to take sequential measurements of the hyperfine structure of a known calibration isotope (generally stable or

¹⁰This assumes no beam polarisation

available in higher yields) before and after performing HF spectroscopy on the desired candidate. Any baseline shift in energy may thus be detected due to variations in the reference HF peak centroids, which are then used to correct for this undesired effect.

3.3 The Data Acquisition System

The DAQ was overhauled during 2010. Under the previous scheme, data collection was triggered by a series of hardware-generated gates (PPC), produced via nuclear instrumentation module (NIM) logic. The gates were manually set to coincide ion/atom bunch passage in the interaction region, and triggered the PMT output, which was recorded to disk.

This gating technique enables background reductions by two orders of magnitude. However, since PMT acquisition only takes place during the gate window, this setup effectively erases any data not covered by the acquisition gate, meaning that events occurring outside that window are not recorded, which represents a serious problem when operating at a facility such as TRIUMF, where access to the various ion sources comes only a few times a year.

To maximise extractable information, the laser spectroscopy group opted to replace the hardware gated DAQ with a continuously running software acquisition system, doing away with timing issues. The new system, known as the multichannel scaler (MCS) is based on a continually running T = 20ns clock which triggers the data acquisition. The new setup, including data collection and voltage control systems is shown in Figure 13.

The voltage applied to the tuning electrodes, just outside the charge exchange cell, where the ions are Doppler shifted into resonance, is controlled by the



Figure 13: Diagram of the acceleration electrode control circuit. The arrow represents processing hierarchy: the DAQ controls the DVM, which goes to the Kepco, which in turn controls the Harrison's final output, while the MCS to DAQ link is bi-directional. The 10000:1 voltage divider (Vdiv) feeds back into the DVM (Digital Volt Meter), controlled by the data acquisition (DAQ), which also records data through the multichannel scaler (MCS) board, connected to the PMT.

combination of two power supplies, which are in turn directly controlled by the data acquisition system computer (DAQ) - which communicates to the amplifiers through the digital volt meter (DVM).

The Kepco is a ×100 amplifier which has a 2000V dynamic range, from -1000 to 1000V, with zero volt crossing capability. The Harrison power supply, with a 0 to 3000V range, adds the Kepco signal to its own floating voltage, outputting the sum to the acceleration electrodes. The Harrison's voltage cannot be remotely manipulated. It is therefore set to a fixed value by hand. To sweep the voltage, it is thus necessary to vary the Kepco voltage. To do this, the DAQ controls the DVM output (a -10 to 10V signal), which is fed into the Kepco. This way, it is possible to sweep the Doppler tuning electrodes over a 2000V dynamic range, with a floating voltage of up to 3000V.

The electrode voltage is also fed back into the DVM, which sends the signal to

the DAQ, storing it to disk. The Doppler electrode voltage is generally in the kV range, above the DVM's input tolerance. Thus, a 10000:1 voltage divider is hooked to the Harrison output, suitably scaling the signal for DVM readings. A data acquisition cycle in the new system is known as a pulsed programmable gate (PPG) cycle. One PPG cycle starts when the ions, after being cooled in the RFQ, are ejected down the CFBS beamline. The cycle ends after a user specified time delay, chosen to ensure the resonance photons have been measured by the PMT.¹¹

Within a PPG cycle, an internal square wave clock on the MCS board periodically triggers PMT acquisition. While this is done, the board logs any incoming PMT counts to disk. These are assigned to time bins based on the clock cycle. Assuming 100 time bins per PPG, and a 50% MCS duty cycle, this would amount to roughly 400 light collection *snapshots* while an ion bunch transits along the beamline.

Once a PPG cycle has completed, the MCS reports to the DAQ, which increments the electrode voltage by a user-specified amount, enabling sweeps across hyperfine resonances.

The PMT has a built in preamp and discriminator pair. Output pulses are of TTL format, with 5 volt amplitudes. The signal is fed directly into the MCS, and is stored in Maximum Integrated Data Acquisition System (MIDAS) files on the DAQ. It is within these files that, for example, PMT output is stored, in the form of time-stamped photon counts. The system is designed to record large volumes of data to file each second, no data processing or analysis that takes place. Consequently, raw output must be post-processed to reconstruct the recorded data in a physically meaningful format.

¹¹Usually the cycle is set to about 200μ s.

At the expense of increased disk space - a relatively small burden - the MCS-DAQ provides the advantage of keeping a broader, more complete record of the experiment, by collecting photons from RFQ ejection to well after the bunch has flown by the PMT.

The full view of the timebunch provided by the MCS allows for rapid identification of any problems with ion delivery or steering. As an example, should a secondary peak emerge a few dozen channels after the principle ion signal, it would be indicative of poor RFQ ejection settings, dividing the ions into two distinct pairs. The former would not be easily identifiable with hardware gating alone.

Generally, the whole experimental cycle of RFQ injection, cooling, ejection and PMT measurement is cycled at 10Hz.

4 Rubidium Hyperfine Spectroscopy

4.1 Physical Properties

Rubidium, of atomic number 37, is the fourth member of the alkali metal group. Discovered in 1861 by both Bunsen and Kirchhoff, it is known for its extreme reactivity with oxygen. In large quantities, great care must be taken to shield it from the atmosphere.

In total, there are 31 known isotopes, from 71 Rb to 102 Rb [15], two of which are commonly found in nature: 85 Rb, with a natural abundance of 72.17% is stable to decay, while 87 Rb, with a half-life of 48 billion years, forms the remaining 27.83% of naturally occurring isotopes.

From a physical standpoint, the Rb family is located almost half way between the Z=28 and Z=50 proton shell closures, while the isotopes stride across the N=50 neutron shell closure, with ⁸⁷Rb being the magic nuclei for N=50, explaining its exceptional half-life. Physically, ⁸⁷Rb has a known charge radius of $r_{ch} = 4.1985$ fm [16].

A neutron sub-shell closure exists at N=56, corresponding to 93 Rb, while deformation is widely believed to exist in the N=60, 62 and 64 subshells [17].

The two closest neighbours to the rubidium isotope family are krypton (Kr) with Z=36 and strontium (Sr), with Z=38. Being in the same intermediate region of the nuclear chart, the chains share similar characteristic features as they all cross the N=50 closure, in addition to the N=56 neutron subshell.

4.2 Previous Rubidium Work

4.2.1 The Thibault et al. ^{76–98}Rb Survey

Much of the spectroscopic work done on the rubidium isotope family has been carried out by Thibault *et al.* at ISOLDE in 1980. In all, they used hyperfine spectroscopy to identify a total of 23 isotopes, in addition to 6 metastable isomers, covering ⁷⁶Rb to ⁹⁸Rb [7] [18].

Ion beam production was accomplished by using the 600 MeV CERN Synchrocyclotron proton source. The various rubidium isotopes were either produced by nuclear spallation upon a niobium target or by the fission of uranium. The reaction products were mass separated by the ISOLDE on-line separator resulting in a mass-selected rubidium ion beam at 60 keV. The ion beam fed into a tantalum target, which was then heated to 1200°C, re-emitting them as thermalized ions through an electrostatically collimated yttrium coated beamline segment, neutralising them in the process. Upon emission from the yttrium tube segment, the atom beam was perpendicularly intersected by a tuneable dye laser beam.

Induced optical pumping of the hyperfine levels, coupled with a hexapole magnet, mass separator and electron multiplier allowed the group to record the hyperfine structure of the isotopes. Thibault *et al.* extracted information including nuclear spin, magnetic moments, quadrupole moments, A & B coefficients, isotope shifts and $\delta \langle r^2 \rangle$ for much of the rubidium chain, as shown in Tables 1 & 2. While the group reported detection of isotopes 74, 75 and 99, yields for the former were below the 10⁵ atoms/s. threshold to which their equipment was sensitive [7]. In spite of this, their work remains the authoritative survey when it comes to the hyperfine properties of the rubidium family.

The terms of equation (2.30), necessary to extract $\delta \langle r^2 \rangle$ from the isotope shift, were obtained from Kopfermann [19], while f(Z) was originally calculated using a formula derived by Babushkin [20], yielding via equation 2.30 a result of -650 MHz/fm², using parameters shown in Table 3. However, recent calculations by Dzuba *et al.* have produced a field shift correction factor of -567.45 MHz/fm² [21], with an uncertainty of 1 %. In light of this, the $\delta \langle r^2 \rangle^{A-87}$ values presented herein were recalculated using the latter. The mass shift was then evaluated using equation (2.29) for each isotope. Since the variation in MSCR is proportional to the field shift only, $\delta \nu_{MS}^{AA'}$ is subtracted from the overall isotope shift prior to conversion according to equation (2.29). The extracted $\delta \langle r^2 \rangle$ are shown in Figure 14.

The magnitude of both the isotope shifts and $\delta \langle r^2 \rangle$ increases on either side of ⁸⁷Rb, strongly hinting at the stability of the N=50 neutron shell closure, even with ⁸⁵Rb displaying a larger MSCR than the former.

As one progresses from ⁸⁷Rb towards the neutron deficient side, an increase in MSCR is apparent, peaking at ⁷⁸Rb, demonstrating the departure from spherical symmetry for the nuclear charge distribution. All reported neutron deficient isotopes, with the exception of ⁷⁶Rb, fill the $1g_{\frac{9}{2}}$ subshell, the latter completing the second available orbital in $2p_{\frac{1}{2}}$.

A	$A(5s^2S_{\frac{1}{2}})$ [MHz]	$A(5p^2P_{\frac{3}{2}})$ [MHz]	$B(5p^2P_{\frac{3}{2}}) \text{ [MHz]}$
76	-701(17)	-18.1(0.5)	36.0(14.1)
77	815.7(5.1)	19.1(1.5)	65.3(3.0)
78			
78^m	1186.8(1.0)	29.4(0.5)	76.5(3.7)
79	2502.0(0.9)	62.0(0.4)	-9.2(2.1)
80	-155.2(3.2)	-1.8(2.3)	32.7(1.9)
81	2557.6(1.7)	63.8(0.8)	37.4(2.2)
81^m	2317.3(0.7)	57.9(0.4)	-69.8(5.4)
82	1031(10)	26.8(3.2)	17.9(6.8)
82^m	563.6(0.9)	14.0(0.6)	94.6(11.2)
83	1061.7(0.6)	26.5(0.4)	18.4(2.1)
84	-1233.7(1.5)	-30.1(0.8)	-1.4(3.3)
84^m	68.2(4.6)	1.2(1.0)	54(26)
85	1011.0(1.0)	25.3(0.4)	21.4(4.0)
86	-1581.2(1.5)	-39.0(0.8)	18.1(3.0)
86^m	563.5(0.3)	14.3(0.4)	34.7(8.9)
87	3415.9(2.0)	84.29(0.50)	12.2(2.0)
88	476.2(2.4)	9.4(2.3)	-1.1(9.0)
89	2960.1(0.9)	72.6(1.1)	13.5(2.4)
90			
90^m	1003.4(0.4)	25.3(0.4)	19.2(4.2)
91	2709.1(1.7)	66.9(1.1)	14.5(2.4)
92			
93	1050.2(1.2)	25.8(0.7)	16.6(3.8)
94	930.4(1.1)	23.2(0.6)	15.3(4.7)
95	993.7(2.5)	24.0(0.9)	19.8(6.1)
96	1365.2(1.6)	32.9(1.3)	23.1(5.3)
97	2286.2(2.6)	55.2(1.8)	54.6(3.1)
98	[0]	-910(10)	

Table 1: A,B coefficients extracted by Thibault *etal*.. Uncertainties are contained in parenthesis, while bracketed values represent tentative assignments. Null entries correspond to spin 0 (HFS-free) isotopes.

A	I [ħ]	$\delta \nu^{A-87} [\mathrm{MHz}]$	Q_s [b]
76	1	-494(17)	0.38(0.15)
77	$\frac{3}{2}$	-498.6(4.5)	0.695(32)
78	0	-478.4(1.5)	
78^m	4	-403.8(1.7)	0.814(39)
79	$\frac{5}{2}$	-391.6(1.5)	-0.098(22)
80	1	-352.8(4.4)	0.348(20)
81	$\frac{3}{2}$	-289.9(1.4)	0.398(23)
81^m	$\frac{9}{2}$	-270.4(1.4)	-0.743(57)
82	1	-233.7(4.2)	0.190(72)
82^m	5	-233.5(3.8)	1.01(0.12)
83	$\frac{5}{2}$	-150.1(1.0)	0.196(22)
84	2	-91.6(2.1)	-0.015(35)
84^m	6	-84(10)	0.57(0.27)
85	$\frac{5}{2}$	-80.1(1.4)	0.228(43)
86	2	-45.8(2.0)	0.193(32)
86^m	6	-32.1(2.3)	0.369(95)
87	$\frac{3}{2}$	0	0.130(21)
88	2	-61.0(5.1)	-0.012(96)
89	$\frac{3}{2}$	-143.7(2.0)	0.144(26)
90	0	-197.7(5.2)	
90^m	3	-188.6(2.0)	0.204(45)
91	$\frac{3}{2}$	-255.8(2.3)	0.154(26)
92	0	-320.4(5.2)	
93	$\frac{5}{2}$	-371.5(2.1)	0.177(40)
94	3	-414.7(2.3)	0.163(50)
95	$\frac{5}{2}$	-495.9(3.8)	0.211(65)
96	2	-528.3(4.8)	0.246(56)
97	$\frac{3}{2}$	-879.7(4.0)	0.581(44)
98	[0]	-910(10)	

Table 2: Nuclear spins, isotope shifts and spectroscopic quadrupole moments extracted by Thibault *etal*.. Uncertainties are contained in parenthesis, while bracketed values represent tentative assignments.



Figure 14: Plot of $\delta \langle r^2 \rangle^{A-87}$ vs atomic number for the rubidium chain. Dotted red lines show positions of different shell closures. Maximum errors are on the order of 1%. Consequently, error bars are too small to be seen by the naked eye.

par.	value	units
$ \psi(0) $	$2.05a_0^{-3}$	m^3
β_s	1.1	Ø
$f(\mathbf{Z})$	-3398	$\frac{MHz}{fm^2}$
${\cal F}$	-650	$\frac{\dot{M}Hz}{fm^2}$

Table 3: List of parameter values used in the computation of equation (2.30) for the isotope shift to $\delta \langle r^2 \rangle$.



Variations in δ (r²) for ⁷⁶⁻⁹⁸Rb, ⁷²⁻⁹⁶Kr and ⁷⁸⁻¹⁰⁰Sr

4.2

Figure 15: Variation in MSCR for the krypton (red), rubidium (blue) and strontium (black) isotope families. Kr displays a similar vibrational pattern in the $1g_{\frac{9}{2}}$ shell [11]. Sr, obtained from [22], shows similar drastic deformation in the N=60 region. Rb $\delta \langle r^2 \rangle$ values are shown in blue for comparison. Maximum errors are on the order of 1%. Consequently, error bars are too small to be seen by the naked eye.

The isotopes ${}^{76-79}$ Rb, from N=39 to 42, lie approximately between the N=28 and 50 neutron shell closures. This can be seen in the trend of $\delta \langle r^2 \rangle$ values, peaking at 78 Rb, indicating the likely presence of vibrational deformation, whose amplitude steadily decreases as the $1g_{\frac{9}{2}}$ shell is filled. This highlights the region of maximal departure from sphericity lying about half way between both magic numbers, and is also visible in the Kr chain, as shown in Figure 15 [23]. MSCR variations for the ${}^{72-96}$ Kr, corresponding to isotopes with N from 36 to 60, are shown in Figure 15, obtained from [11].

Meanwhile, on the neutron rich side, rapid and approximately linear growth covers the isotopes ${}^{88-93}$ Rb, as neutrons begin to fill the unoccupied $2d_{\frac{5}{2}}$ neu-

tron subshell which possesses 6 degenerate states. A slight disruption in the trend for $\delta \langle r^2 \rangle$ may be seen for ${}^{94-96}$ Rb, coinciding with occupation of the $1g_{\frac{7}{2}}$ subshell.

A drastic increase in MSCR then occurs, between $^{96-97}$ Rb, roughly 10 times the rate of increase from the previous 8 isotopes. This jump is indicative of strong deformation. The departure from sphericity may be seen in the change in Q_S values between $^{96-97}$ Rb, where the quadrupole moment increases rapidly, representing the largest inter-isotope jump on the neutron rich side. MSCR variations obtained by Buchinger *et al* [22] for the strontium isotopes are also shown in Figure 15, displaying a similar jump in charge radius at the N=60 locus. The strong variation in $\delta \langle r^2 \rangle$ in both the Rb and Sr isotopes at N=60 suggests the presence of a rotational band [17], severely affecting the shape of the charge distribution. In addition, FRDM¹² computations by Moller *et al.* [25] have indicated that several deformation modes coexist in the N=60 region, with both prolate and oblate spherical deformations being extremely close in energy for the nuclear potential, within 1 MeV.

From another perspective, theoretical work done by Campi & Epherre using density dependent Hartree-Fock [24] also hints at this behaviour in the Rb chain. The authors have tabulated β_2 values for the adjacent Kr and Sr isotope chains, from N = 38 to N = 68, shown in Figure 16. The overall β parameter behaviour does indicate the presence of deformation beyond the N = 56 subshell closure, with extremely close agreement between the Kr and Sr cases.

The mean field computations consistently underestimate $\beta_2 \sim 0$ in the neutron deficient region. This is attributed to the pronounced vibrational spectra of

¹²Finite Range Droplet Model



Theoretical and Experimental B₂ Values for Kr and Sr Isotopes

Figure 16: Theoretically computed density dependant Hartree-Fock (DDHF) & experimentally extracted values of β_2 for the Kr and Sr isotope chains, obtained from [24].

isotopes in the region, in particular to zero-point quadrupole vibrations ($\lambda = 2$) in the ground states of the isotopes, which were not reproduced by the DDHF model. Nevertheless, inclusion of experimentally extracted β_2 values from spectroscopy indicate the presence of strong deformation, equal in magnitude to the neutron rich case, peaking at or around N = 40 [24].

4.2.2 ^{74–78}Rb TRIUMF Survey

The TRIUMF laser spectroscopy group undertook a survey of the neutron deficient rubidium isotopes in late 2010. The investigation covered the isotopes $^{74-76}$ Rb, using 78m,78 Rb as a frequency standard. The inclusion provided overlap with Thibault *et al.* data. The experiment extracted spectroscopic moments from previously unobserved rubidium isotopes, namely 74,75 Rb, providing information on the MSCR at the proton drip line, which happens for N=Z in the case of rubidium.

The isotopes were produced by bombardment of a 98 μ A p^+ current onto a niobium foil target. The Rb ions were electrostatically delivered to the RFQ with an energy of 28 keV, after which they were injected into the RFQ for 80ms and cooled by interaction with He buffer gas for 1ms. The cooled and bunched ions were then ejected down the beamline, against the collinear laser tuned slightly off of the D_2 line with $\lambda = 780$ nm. For this, the RFQ's entrance electrode was lowered for 100μ s, giving all the ions sufficient time to escape. The overall RFQ cooling process was repeated at 10Hz [16].

Yields for the studied Rb isotopes are displayed in Figure 17. While the ⁷⁸Rb yields were similar to those of ISOLDE 30 years prior, isotopes 74-76 all displayed increases of an order of magnitude, with ⁷⁴Rb being the lowest yielding isotope at 1.7×10^4 ions/s. The ions were Doppler shifted into resonance with the laser, immediately prior to neutralisation by Na vapour in the charge exchange cell, heated to 445°C. Neutralisation efficiency was measured to be $50\% \pm 10\%$.

The PMT used to record de-excitation photons was fitted with a red colour filter to avoid counting any scattered laser light. Overlap between the ion



Figure 17: ISAC yield database measurements for production yields of neutron deficient rubidium isotopes by 500 MeV p^+ spallation upon a niobium (Nb #5 HP) target, TRIUMF [14].

beam and the laser was ensured by using retractable aluminium apertures of 3 mm and 1 mm, in sequence. The former were aligned with the laser first, then the electrostatics in the beamline were adjusted. The 3mm ensured a coarse tune, while the 1mm was used for finer adjustment. With this procedure complete, the apertures were removed and data collection began. PMT data acquisition was accomplished by using three separate hardware gates¹³, creating observation windows which were made to coincide with the predicted time of ion bunch passage within the interaction region. The gates consisted of two 4μ s gates, one μ s apart, and of a larger 12μ s gate, which covered both. This ensured PMT acquisition overlapped with the passage of the cooled Rb bunch. The experimentally gathered spectra are shown in Appendix A.

 $^{^{13}\}mathrm{Note}$ that this run took place prior to DAQ overhaul.



Figure 18: Plot of $\delta \langle r^2 \rangle^{A-87}$ vs neutron number for the neutron deficient isotopes $^{74-78}$ Rb, measured at TRIUMF. The reference isotope was 78 Rb. Error bars are too small to be seen by the naked eye.

Nuclear spin information was known for ⁷⁶Rb, with I=1, while ^{78,78m}Rb had previously assigned values of I=0 and 4, respectively. Studies of the β and γ decay mechanisms of ⁷⁵Rb had previously constrained the nuclear spin values to either I= $\frac{3}{2}$ or $\frac{5}{2}$ [26] and [27], while ⁷⁴Rb was known due to its role in superallowed beta decay[16].

Application of equations (2.16)-(2.19) to collected TRIUMF spectra produced isotope shifts and nuclear spins for measured isotopes, and are shown in Table 4. For the isotope shift to $\delta \langle r^2 \rangle$ computations, a new Dzuba *et al.* value was used. Further, the specific mass shift was set to zero, as done in the work of Thibault *et al.*. The values for both isotope shifts and changes in MSCR are presented in Table 5 and shown in Figure 18.

А	I [ħ]	$A(5s^2S_{1/2})$ [MHz]	$A(5p^2P_{3/2}) \text{ [MHz]}$	$B(5p^2P_{3/2})$ [MHz]	χ^2
74	0				0.93
75	3/2	719.6(10)	17.8(01)	63(27)	1.18
75	5/2	478.1(10)	11.9(02)	85.5(22)	1.87
76	1	-693(08)	-17.15(02)	32(07)	1.08
78	0				0.83
78^m	4	1185.1(05)	29.3(01)	83.1(22)	0.76

Table 4: Nuclear spin assignments, hyperfine moments and χ^2 goodness-offit test for $^{74-75-76-78m-78}$ Rb, obtained by E.Mane *et al.*. 75 Rb shows two separate sets of parameters, based on differing initial assumptions for nuclear spin. For the former, I=3/2 is concluded to correspond to the nuclear spin, based on the χ^2 results.

А	$\delta \nu^{A-87} [\mathrm{MHz}]$	$\delta \langle r^2 \rangle^{A-87} [\text{fm}^2]$
74	-379(10)	-0.04(5)
75	-518(5)	0.26(5)
76	-501(4)	0.30(5)
78	-478(2)	0.37(4)

Table 5: Isotope shifts and changes in MSCR with respect to 87 Rb of the ${}^{74-78}$ Rb isotopes. Uncertainties are shown in parenthesis. Note that the values of $\delta \langle r^2 \rangle^{A-87}$ were computed using the field shift correction factor of Dzuba *et al.* from [21].

Comparison of $\delta \nu^{78-87}$ with the quoted value in Table 2, of Thibault *et al.* shows agreement between both shifts, therefore charge radii, within error bars.

4.3 Neutron Rich Rubidium Program at TRIUMF

4.3.1 Background

With hints of significant rotational deformation in the neutron rich end of the rubidium chain, as can be seen by the sudden $\delta \langle r^2 \rangle$ jump beyond ⁹⁶Rb, obtaining high precision hyperfine spectra for isotopes in the region is a goal for the TRIUMF laser spectroscopy group.

The spectroscopy is part of a two-tiered study of rubidium being carried out in the ISAC-I facility, in conjunction with the 8π group. The latter will concurrently perform β -decay spectrometry using a spherical array of high purity germanium (HPG) detectors, in addition to tracking e^+e^- pair production and annihilation using an array of organic scintillator tiles [28].

Based on 2010-2011 measurements from the UCx target, listed yields for the heavy rubidiums at and beyond A=98 are shown in Figure 19, in addition to the frequency reference isotope, 92 Rb.

From the laser spectroscopy perspective, another interesting prospect is the identification of possible metastable isomers for 98,99,100 Rb, whose presence has been inferred by experimental observations of β -decays, in addition to theoretical computations in both [29] and [15]. Reference ground states and isomers, with selected properties, are shown in Table 6.

The first experimental run was scheduled during December 2011, with the aim of studying the heavy end of the Rb chain, specifically to obtain the first TRIUMF spectra for the reference isotope 92 Rb - possessing a known hyperfine-structure-free D_2 line due to its spin-0 nucleus. In addition, preliminary searches were performed for the heavy isotopes, listed in Table 6. This served as an energy reference, as detailed in Section 2.



Figure 19: ISAC yield database measurements for production yields of heavy rubidium isotopes by 500 MeV p^+ spallation upon a uranium carbide target (UCx #1), TRIUMF [14].

AX	$T_{1/2}$	$\Delta E \ [keV]$	I [ħ]	Decay Mode / Rel. Intensity (%)
92 Rb	$4.492~\mathrm{s}$	0	0	β^- : 100, β^- n: 0.0107
$^{98}\mathrm{Rb}$	$114~\mathrm{ms}$	0	(0,1)	$\beta^-:$ 100, $\beta^-\mathrm{n}:$ 13.8
$^{98m}\mathrm{Rb}$	$96 \mathrm{ms}$	290(130)	(3,4)	β^- : 100
$^{99}\mathrm{Rb}$	$50.3 \mathrm{\ ms}$	0	$\frac{5}{2}$	β^- : 100, β^- n: 15.9
$^{100}\mathrm{Rb}$	$51 \mathrm{ms}$	0	(3,4)	β^- : 100, β^- n: 5.6
100m Rb*	N/A	N/A	(6)	N/A

Table 6: Selected list of neutron rich rubidium isotopes as computed by the Nubase-2003 Evaluation of Nuclear and Decay Properties [29], including the 92 Rb frequency reference. *- The 100m Rb isotope, with unknown properties apart from nuclear spin, is listed on the Brookhaven Nuclear Data Table - NuDat 2.6 [15].

4.3.2 $\delta \nu$ and Centroid Computation

To facilitate the experimental survey, predictions were made for the values of both the isotope shifts and hyperfine peak energies of the isotopes listed in Table 6.

Isotope shift values were obtained by performing a clamped cubic spline interpolation of the values reported by Thibault *et al.*, listed in Table 4, via MATLAB. The interpolated function was then smoothly extrapolated using a monotonically decreasing second degree polynomial which uses a smoothnessof-derivative criterion on the endpoints of the spline, for values up to A=105. The extrapolated polynomial fit is shown in Figure 20.

The generated function was used to obtain isotope shift predictions for isotopes ^{99,100}Rb. The results are listed in Table 7.

Centroid energies for the hyperfine peaks were then computed using equations (2.16) & (2.17), using the listed spin assignments shown in Table 6, as well as the beam energy, set to 20 keV. Values for the A coefficients, unknown for 99,100 Rb were estimated by linearly interpolating beyond the values for 97,98 Rb, while the B coefficients were set to zero, due to the weaker dependence on the latter in equation (2.16). While this assumption might seem crude, it is worth noting that in the case of rubidium, due to the relatively small scale of the

AX	$\delta \nu^{A-87} [\mathrm{MHz}]$
98 Rb	-932.3
$^{99}\mathrm{Rb}$	-1036
$^{100}\mathrm{Rb}$	-1111

Table 7: List of extrapolated isotope shift values for the heavy rubidium isotopes. Note that 98 Rb is presented for completeness, already being part of the interpolation set.



Figure 20: Extrapolated quadratic polynomial obtained by clamped cubic spline interpolation of the isotope shifts for the rubidium isotopes reported by Thibault *et al.*. The MATLAB extrapolation algorithm uses a smoothness condition on the endpoints of the interpolating polynomial, to ensure a smooth and monotonic progression of the data.

HFS, with splittings on the order of about one GHz, varying the value of the A coefficient by an order of magnitude will result in an energy shift on the order of tens of volts, of the voltage applied to Doppler tune the ions into resonance. In addition, typical experimental sweeps cover from 200 to 1000V, easily making up for the resulting uncertainty. The HFS computation produced the absolute energy of the hyperfine peak position, that is, the HFS centre of mass frame splittings, added to the overall beam energy. From this, it is possible to determine both the optimal Harrison power supply (see Figure



Figure 21: Predicted energies of the hyperfine peaks for $^{92,98-100}$ Rb in absolute energy space. Note that isotopes with the same A value are intentionally displaced by A = 0.25 relative to each other for clarity. Since the ions are positive, setting the Harrison negative allows one to sweep an extra 3000 eV, while the Kepco can remove 1000eV. The effective range is thus from 19,000 eV to 22,000 eV.

13) polarity¹⁴ in addition to the laser wavenumber. The latter's selection was done to place all of the predicted peaks within the cell voltage scan region. The computation results, shown in Figure 21, constrained the cell voltage to be negative.

4.3.3 Equipment Setup

For optimal ion neutralisation, the charge exchange cell was fitted with natural rubidium, instead of the more frequently used ²³Na. While both elements are members of the Alkali metal group, with closely matched structures, the rubidium vapour's ionisation potential necessarily corresponds very closely to that

¹⁴Recall that the Harrison, on floating ground, cannot cross zero and has a 3000V range.



Figure 22: The diode laser (blue box) mounted on an optics table. The beam is steered, via mirrors and lenses, to the yellow optical fibre line, which takes the laser light to the vacuum beamline.

of the ions. The cell was heated to a temperature of 253.2°C and the resulting neutralisation efficiency was estimated to be over 0.8 by MCP measurement. A Toptica diode laser was used as primary light source, shown in Figure 22. The laser was locked at a wavenumber of 12807.9894 cm⁻¹ (781nm) by using an in-house laser locking feedback system.

Frequency drifting was countered by feeding the output laser signal, in addition to a temperature stabilised HeNe laser into a Fabry-Perot etalon [30].



Figure 23: Imaging of the stabilised diode laser beam profile captured by overhead CCD. Image scale is displayed for reference.

The stabilised laser signal was then fed via optical fibre into the beamline. Focusing and centring of the former was accomplished by tuning a series of optical elements including telescope lenses and reflective mirrors. The laser profile was temporarily reflected onto an overhead CCD to measure the quality of its focus. This is shown in Figure 23. Imaging software coupled to the device was used to determine that the beam's diameter was ~ 2.6 mm.

To prevent unnecessary PMT counts in the event of ion signal loss, either due to vacuum degradation or proton beam trip, a coincidence measurement was set up. Residual ions (negligible but nevertheless measurable) were deflected on to an off-axis MCP located beyond the interaction region by a set of quadrupole deflectors. The MCP signal, indicating ion beam presence, was then fed into a discriminator in addition to the RFQ's ejection signal. The resulting logic signal was fed into the DAQ and recorded to disk. Although standard procedure calls for a run stop in the event of beam loss, if this were to be missed, the logic signal produced an effective way to clean up the data, removing background photon counts acquired in absence of beam.
Run no.	A [Counts]	$\mu \; [\mathrm{MHz}]$	σ [MHz]
672	95(23)	-1194.62(0.76)	13.4(3.9)
679	42(18)	-1205.1(3.0)	57(14)
684	89(12)	-1221.0(1.6)	26.4(4)
685	91(18)	-1226.1(1.3)	17(14)
686	57.8(9.6)	-1225.41(1.4)	33.8(2.6)
697	226(15)	-1219.29(0.80)	26.5(2.6)
710	42.5(8.7)	-1216.3(1.5)	32.6(2.9)

Table 8: List of returned fit parameters for the 92 Rb single hyperfine peak. Fitting was performed via Root-MINUIT [31]. Note the large centroid shift (μ) between runs 672 and 679.

4.3.4 Results & Discussion

The beam energy was measured as 20000 eV by the ISAC operations group. After beamline tuning was completed with 238 U, measurements for 92 Rb were performed, with an RFQ injection time of 100ms.

In total, 7 separate spectra for 92 Rb were recorded, at various times during the two day experiment. A selection of these, in addition to fitted Voigt functions, are shown in Figure 24. Extracted centroids and peak widths are plotted as a function of time in Figure 25. As 92 Rb is a spin-0 nucleus, there are no hyperfine moments to extract.

The extracted fit parameters are shown in Table 8. Since 92 Rb corresponds to the calibration isotope, only changes in its centroid frequencies are meaningful. Inspection of the centroid values shows that they suffered an energy drift whose maximum amplitude was of 31.4 ± 2.1 MHz, which in the case of 92 Rb corresponds to a baseline voltage change of approximately 5 volts. In addition, the widths display nontrivial variation which could indicate variation in the beam delivery energy.



Figure 24: Selected spectra for 92 Rb obtained at the TRIUMF CFBS experiment. Laser wavenumber was set to 12807.9484 cm⁻¹. Note that x-axis values have been normalised to the $\lambda = 780.241$ 209 686 nm 87 Rb D_2 line.



Figure 25: Plot of extracted centroid μ and peak full width at half maximum (FWHM = $2\sigma\sqrt{2ln(2)}$) versus time of recording. T = 0 corresponds to the start of the experiment. Note that runs 684-686 have been averaged, as they were each taken 10 minutes apart.

With the 92 Rb data acquisition successful, several attempts were made to record the spectrum of 98 Rb. Yields for the former, measured on an MCP beyond the interaction region, were estimated to be one fifth that of 92 Rb. RFQ injection time was increased to 250ms. It was not possible, due to both low ion yields and tuning issues, to obtain the hyperfine spectrum of 98 Rb. Several scans, covering a region of approximately 8,000V or 20,000MHz were performed, with no traces of the isotope. A histogram of all 98 Rb scans is presented in Figure 26. Due to different scan times, different regions have uneven background levels. However, judging by the width of the 92 Rb peaks in Figure 24, whose 1/e cutoffs are approximately 200 MHz apart, with signalto-noise ratios of at least 5 (run679), a 98 Rb peak should clearly stand out of the background, given the scan durations, on the order of 2 to 4 hours each.



Figure 26: Composite scan spectrum showing PMT counts vs frequency for all 98 Rb scan attempts. For these, the laser was set at a wavenumber of 12807.9484cm⁻¹. Histograms were binned at 100MHz per bin. Note that different background levels correspond to different counting times.

Figure 27 shows the [-6,0] and [3,7] GHz regions, rebinned at 20 MHz. No clear, structured peaks can be unambiguously discerned in either.

Approximately 20 hours into the experiment, shortly after the first ⁹⁸Rb data acquisition run had begun, the ion signal was lost due to an unknown event. Significant troubles were encountered re-acquiring the beam, which required several hours of re-tuning with both the ²³⁸U and ⁹²Rb. It is believed the UCx target geometry suffered a slight thermally induced shift. The former would perturb the output energy of the isotopes. After re-tuning the beam down to the RFQ, there would be no way to discern this shift in energy. In particular, inspection of both the centroids and peak FWHM values in Figure 25 shows both varying considerably for the first 23 hours of data acquisition. This is strongly indicative of a change in baseline beam energy, and the much more drastic variation in this time interval lends credence to the outlined hypothesis. The exact cause of this problem is being investigated.

The measurement of ⁹²Rb which will serve in subsequent investigations of longer duration as the reference isotope, was successfully achieved. The electrostatic transmission tunes through the beamline were noted, in addition to vapour cell temperature and Harrison polarity settings. As such, it will be possible to rapidly reproduce the tune during future runs, allowing the group to begin acquisition promptly.



Figure 27: Composite scan spectrum showing PMT counts vs frequency for 98 Rb [-6,0] & [3,7] GHz ranges. For these, the laser was set at a wavenumber of 12807.9484cm⁻¹. Histograms were rebinned at 20MHz per bin. Note that different background levels correspond to different counting times.

5 Spectroscopic Data Analysis Tools

5.1 The Root Analyser & MIDAS Files

The program HInSane is constructed around the program Root-Analyser, developed for the laser spectroscopy group by the TRIUMF-DAQ group. The function of Analyser itself is to convert MIDAS¹⁵ .mid files to .root, the former containing raw experimental data such as PMT counts, while the latter is suitable for analysis and processing. The Analyser, called in console as anaPol, has two independent modes of operation: online and offline. The raw output upon which Analyser operates is shown in Appendix B.

Online mode allows for real-time conversion of output experimental data during MCS data acquisition. The analyser is thus written to dynamically allocate memory and access the output data before it is written to file. Conversely, offline mode requires a specified input file (.mid), from which it will produce the same set of conversion routines. While both modes have their own specificities, they do share a similar structure, always seeking the PMT raw data in the MIDAS stream. A brief outline of analyser's routines are shown in Figure 28.

 $^{^{15}\}mathrm{Maximum}$ Integrated Data Acquisition System



Figure 28: Overview of the original Root-Analyser. The processes presented correspond to C++ subroutines, in the order of operation present in the source code. Within main, two separate operation modes exist, being the online and offline modes, allowing for data processing during data collection, or from a midas file. The ultimate output of the program is a set of Root histograms displaying the data. In offline mode, the MIDAS-to-Root conversion is done within a while loop, operating indefinitely until an end-of-file trigger. Note that the hexadecimal values 0x8000 and 0x8001 in midas format are taken to signify beginning/end of run (BOR/EOR), respectively. Within the midas file, events for which the midas variable eventID is 5 correspond to raw data.

5.2 HInSane - A Spectroscopic Data Analysis Package

HInSane will perform the exact same operations as the original Analyser, in addition to the following functions:

- Increasing the signal to noise ratio (SNR) by integrating only photons within the time bunch
- Fitting the resulting spectrum's HFS with Voigt peaks
- Extracting relevant physical coefficients arising from the spectrum fit

The user must enter a group of input parameters, in the form of a template file known as parameters.dat, which is read by HInSane. In Figure 28, all of the extra HInSane routines take place after MIDAS to Root conversion has taken place. This way, HInSane is capable of performing all functions performed by Analyser, in addition to the analysis and noise reduction.

The complete list of user input parameters is shown in Table 9. This file provides the program with experiment properties such as the isotope mass, nuclear spin, RFQ voltage, laser wavenumber and so on. All of these variables will be used in subsequent computations. The file must be located in the same directory as the program executable.

All files or folders produced by HInSane are stored in a folder named output#, where the pound sign corresponds to the file number. This folder (the main folder) is automatically created in the same directory from which HInSane is executed.

With the conversion out of the way, the program may now begin its core group of functions, namely spectroscopic data analysis. The raw output of the midas file consists of a two dimensional histogram plot featuring acceleration voltage

Par.	Par. Description	Units	Par.	Par. Description	Units
1	Atomic Number	Ø	12	λ_{D2}	cm^{-1}
2	Atomic Mass	amu	13	λ_{laser}	$\rm cm^{-1}$
3	Ι	\hbar	14	BI_{left}	timebins
4	J_{low}	\hbar	15	BI_{right}	timebins
5	J_{high}	\hbar	16	Output File Count	Ø
6	V_{RFQ}	V	17	σ -left	timebins
7	А	MHz	18	σ -right	$\operatorname{timebins}$
8	$\frac{A}{A'}$	Ø	19	PMT reject level	PMT counts
9	B	MHz	20	Gauss or Voigt	Ø
10	B'	MHz	21	Partial Spectrum?	Ø
11	FWHM	MHz	22	Isotope Shift	MHz

Table 9: List of parameters found in the file parameters.dat. Parameters 7-10 are the HF A,B coefficients. BI stands for bunch interval and FWHM corresponds to the peak Full Width at Half Maximum.

as y-axis (displayed as DAQ channel step), timebins on the x-axis and PMT counts as the z-axis. A 2D example X-Y projection Root file obtained during a ²³Na run is shown in Figure 29.

The HFS of the $S_{\frac{1}{2}}$ ground state for ²³Na D_2 line may be seen, in the form of two Doppler widened peaks which span the x-axis from approximately 25 to 40 μ s. The position of the peaks reveal the profile of the timebunch crossing the interaction region. Note that the displayed scan is too coarse to show the hyperfine multiplets. Should a hardware gate have been used, it would have been crucial to tune it to this exact region to successfully record the data.

The package next produces a series of slices both along the x and y-axes, allowing inspection of PMT readback, individual bunch profile characteristics and data quality. All of these are stored in separate folders. The bunch profiles are generically named timedat#.dat, indicating the DAQ-step (energy) of the particular scan.



Figure 29: HInSane raw converted output of PMT counts, obtained during a $^{23}\mathrm{Na}$ run at TRIUMF.

The frequency files, corresponding to slices at constant time, are stored as freqdat#.dat, numbered according to the timebin number at which the projection is taken.

5.3 Channel to Frequency Space Conversion

To make the data physically relevant, it is necessary to convert the x-axis into an energy-dependent quantity. While there are many possible choices for this conversion, it was decided to write HInSane such that the x-axis represents the Doppler shifted laser frequency, as seen in the frame of the ions in the beamline interaction region.

The first step necessary to accomplish this conversion is the extraction of the



Figure 30: Graph representing the acceleration electrode (Kepco+Harrison) voltage per channel in the MCS. The bottom residual plot shows the difference between the quoted fit function and the recorded Kepco ramp.

voltage to channel curve, saved in the raw file. This linear relationship is shown in Figure 30.

The slope of the linear function thus represents the voltage scan carried out during the run. The scan ends when it reaches the end of the line, at the discontinuity. With this in hand, it is possible to convert channels into an energy compatible unit, such as frequency.

Root is called by HInSane to perform a linear fitting of the slope in Figure 30:

$$y = mx + V_0 \tag{5.1}$$

The slope parameter m has units of volts/channel, while the offset parameter V_0 represents the Harrison offset voltage. The returned fit parameters are then

multiplied by 10,000, restoring their pre-voltage divider values.

The channel-to-frequency conversion then proceeds, by taking into account the Doppler shifted laser frequency viewed in the ions frame of reference. First, the relativistic β parameter of equation (2.26) is determined, through use of equation (5.1):

$$\beta = \sqrt{2 \frac{E_{beam} - (mx + v_0)}{E_{mass}}} \tag{5.2}$$

Where x represents the integer channel number and:

$$E_{mass} = (931.494061 \times 10^6) m_{amu} \tag{5.3}$$

is the ion mass energy equivalent value, in eV. m_{amu} represents the ion mass in atomic mass units (amu). The conversion then concludes by computing the Doppler shifted frequency:

$$\nu = (2.99792 \times 10^4) \lambda_{laser} \sqrt{\frac{1+\beta}{1-\beta}} - \lambda_{D2}$$
(5.4)

Note that in equation (5.4) both λ_{laser} and λ_{D2} are in units of MHz. Further, the frequency is presented relative to the D₂ line of the atom in question. equation (5.4) is completely analogous to equation (2.25) and represents the final converted axis displayed on all frequency space graphs returned by HInsane.

5.4 Timebunch Shape and Fitting

One of the most important function of HInSane is to fit the shape of the timebunch. Doing so allows quantitative assessment of the mean time of arrival and duration of the bunch in the interaction region. If this is defined, it is then possible to exclude all data which lie before and after bunch interaction.



Figure 31: Typical MCS timebunch profile, obtained during a 23 Na run. In this particular case, one timebin is 2μ s wide.

The timebunch possesses a skewed shape, as can be seen in Figure 31, rendering the fitting process slightly more challenging. This is attributable to the RFQ kicker voltage and potential well shape. The result is that higher energy ions in the RFQ are ejected swiftly and are thus closely spaced within the beamline. The bunch leading edge thus arrives with more spatial coherence in front of the PMT - the signal goes from background to peak in less than 15 channels. However, ions with less energy will exit the RFQ with lower velocity, or may exit the RFQ a few μ s after the kicker switches on. The end result is that the trailing edge of the ion bunch contains a mix of lower energy and delayed ions, which possess less spatial coherence. Again in Figure 31, it is apparent that the trailing end signal lasts up to 50μ s, about 3 times longer than the leading edge.

The first step in the fitting routine begins with a regular Gaussian fit, using

the standard form defined in equation (2.23). The user is required to enter a preliminary time interval where the timebunch is expected to lie - the BI parameters in Table 9. This interval may be much wider than the actual bunch width, so long as it is entirely contained within its confines.

The first fit will be quite poor due to the skewedness of the signal. MINUIT, Root's fitting algorithm, will either *tack on* the Gaussian to the leading or tailing edge, resulting in an under or overestimated width. However bad the fit parameters are, they are nevertheless used as first-guess values for a more refined fit function, which matches the skewed bunch profile.

The function in question is known as an Exponential Gauss Hybrid (EGH) function, which consists of a Gaussian convoluted with an exponential, of decay constant τ . Algebraically, it may be defined as follows [32]

$$f(t) = A_0 exp\left(\frac{-(t-\mu)^2}{2\sigma^2 + \tau(t-\mu)}\right).$$
 (5.5)

As in the Gaussian case, the EGH is scaled by the constant A_0 . However, the following constraint is imposed:

$$2\sigma^2 + \tau(t - \mu) > 0 \tag{5.6}$$

Upon inspection, equation (5.6) dictates a domain constraint upon equation (5.5) - it is forced to zero before a specified value of t. Indeed, as τ - the exponential decay constant - decreases, the time domain of equation (5.5) decreases as well, being forced to start at higher and higher time values. This is merely a consequence of the asymptotic nature of the time-decaying exponential function.



Figure 32: Measured timebunch profile and exponential Gauss-Hybrid (EGH) fit obtained during a 23 Na run at TRIUMF. Note the EGH discontinuity in the first two timebins. See equation (5.6) for details.

However, given the nature of the experimental setup, the RFQ's operational characteristics and the distance between RFQ and PMT in the CFBS beamline, the timebunch will always be situated around a mean value sufficiently large in time-space to ensure fitting problems never arise.

As an example, for the ²³Na data series collected with the MCS, typical EGH fits return values for τ between 4 and 7 timebins, meaning that by equation (5.6), the EGH is defined for t $\gtrsim 10\mu$ s. With the mean timebunch arrival generally in the neighbourhood of $\mu \approx 60\mu$ s, well away from the domain cutoff. The profile of the timebunch, as well as the fitted EGH are both shown in Figure 32.

5.5 PMT Count Integration

The EGH fit produced by MINUIT produces a set of five fit parameters, corresponding to those in equation (5.5). These parameters provide a statistically meaningful definition of the location and shape of the timebunch signal, which is crucial for successful analysis is to be attempted on the former.

HInSane's next goal is then to attempt a further reduction of background, by integrating all PMT counts located under the area of the timebunch, rejecting anything that lies before or after the ion bunch crossed the PMT - counts mainly attributable to light reflection within the beamline or PMT dark counts. The fundamental reference for the integration operation is the mean μ returned by the EGH, which is rounded to the nearest integer to reflect the discretised, binned nature of the PMT count time spectrum.

Integration proceeds by summing up PMT counts around the mean. The extent of the integration is left to the user as two variables in parameters.dat, posed in terms of so-called sigma bounds: the number of Gaussian standard deviations over which the integral will span both to the left and right of μ . It is important to note that although the EGH presents an asymmetric profile, the mathematical significance of σ remains the same as for a classical Gaussian - in absence of any exponential skewedness, the standard deviation parameter would be symmetric about the central point of the function.

Robust values for the σ -bounds have experimentally been found to correspond to 2σ to the left and 3.5σ to the left - this produces an integral that spans *all* of the EGH profile.

Based on user specified input, n files are produced, labelled freqintegral < n > .dat. File number 1 integrates over $\frac{1}{n}$ of the asymmetric bounds of the EGH, with



Figure 33: Graphical representation of the integration files. Horizontal grey rectangles represent the integration domain. Bins spanned by a rectangle are fully integrated in the files designated by the numbers 1-10. The red bin marks the position of the fit mean.

each integer step reaching out further by the same amount. The last file features full integration, out to the bound values.

Figure 33 shows the result of the integration routine, for 2σ to the left and 3.5σ to the right. This particular timebunch was obtained during a ²⁰⁸Fr run.

5.6 Hyperfine Spectrum Simulation

With the provided nuclear spin in parameters.dat, along with the J_1 and J_2 values, HInSane computes a simulated HFS for the isotope in question¹⁶, by computing the theoretical coupling strength between hyperfine levels.

The spectrum simulation is based on the assumptions of Russell Saunders

 $^{^{16}\}mathrm{Credit}$ to the original MATLAB implementation goes to Prof. John Crawford, McGill University. The routine was extensively modified and re-written in C++ by the author of this thesis.

(LS) coupling, which postulates that L and S are good quantum numbers. In other words, both vectors must be linearly independent such that they may be added vectorially into the composite vector \vec{J} , as is the case in Russell Saunders coupling.

This assumption will remain valid so long as the electrons are not subjected to powerful external magnetic fields, which does not happen in this experiment. The application of Russel-Saunders coupling rules and equations to the HFS of spectral lines then follows by a substitution of quantum numbers:

$$\begin{array}{ccccc} L & \rightarrow & J \\ S & \rightarrow & I \\ J & \rightarrow & F \end{array} \tag{5.7}$$

Effectively, this stipulates that the quantum numbers I and J are perfectly analogous to L and S.

The spectrum simulation then starts by defining an m by n matrix \mathcal{T} , where $m = I + J_1$ and $n = I + J_2$, J_1 and J_2 corresponding to the lower and upper electronic states, respectively. Each slot represents a possible electronic transition in the isotope, as measured with the quantum number F = I + J. The matrix \mathcal{T}_{mn} represents the relative coupling strength between both F states in the electronic arrangement, in other words the relative transition probability. The level couplings are then computed according to six distinct possible cases, consisting of two sets of three depending on the $J_1 \rightarrow J_2$ transition, as shown in Figure 3 . For Δ J \neq 0, the three couplings are: F–1 \rightarrow F:

$$\mathcal{T}_{mn} = \frac{(J_2 + n + I + 1)(J_2 + n + I)(J_2 + n - I)(J_2 + n - I - 1)}{|J_2 - I| + n - 1}$$
(5.8)

 $\mathbf{F} \to \mathbf{F}:$

$$\mathcal{T}_{mn} = -(J_2 + |J_2 - I| + n + I)(J_2 + |J_2 - I| + n - I - 1) \times \frac{(J_2 - |J_2 - I| - n + 1 + I)(J_2 - |J_2 - I| - n - I)(2|J_2 - I| + n)}{(|J_2 - I| + n - 1)(|J_2 - I| + n)} (5.9)$$

 $F+1 \rightarrow F$:

$$\mathcal{T}_{mn} = (J_2 - |J_2 - I| - n + I + 1)(J_2 - |J_2 - I| - n + I) \times \frac{(J_2 - |J_2 - I| - n - I)(J_2 - |J_2 - I| - n - I - 1)}{|J_2 - I| + n}$$
(5.10)

By only ascribing nonzero probabilities to these three possible F transitions, the electronic selection rules:

are effectively enforced. On the other hand, for $\Delta J = 0$, the elements of \mathcal{T}_{mn} take the values:

 $F-1 \rightarrow F$:

$$\mathcal{T}_{mn} = -(J_2 + |J_2 - I| + n - I)(J_2 + |J_2 - I| + n - I - 1) \times \frac{(J_2 - |J_2 - I| - n + I + 2)(J_2 - |J_2 - I| - n - I + 1)}{|J_2 - I| + n - 1}$$
(5.11)

 $\mathbf{F} \to \mathbf{F}:$

$$\mathcal{T}_{mn} = \frac{2[J_2(J_2+1) + (|J_2-I|+n-1)(|J_2-I|+n) - I(I+1)](|J_2-I|+n)}{(|J_2-I|+n-1)(|J_2-I|+n)}$$
(5.12)

 $F+1 \rightarrow F$:

$$\mathcal{T}_{mn} = -(J_2 + |J_2 - I| + n + I + 1)(J_2 + |J_2 - I| + n - I) \times \frac{(J_2 - |J_2 - I| - n + I + 1)(J_2 - |J_2 - I| - n - I)}{|J_2 - I| + n}$$
(5.13)

All elements of \mathcal{T}_{mn} are then normalised to the largest coupling, which is given a value of 100.

Next, HInSane computes the level transition energies for all possible electronic transitions given J_1 , J_2 and I. The program proceeds by first declaring two vectors \mathcal{L}_m and \mathcal{U}_n , corresponding to the lower and upper electronic state energies, respectively:

$$\mathcal{L}_m = \frac{A\frac{C}{2} + \frac{B}{4} [\frac{3}{2}C(C+1) - 2I(I+1)J_1(J_1+1)]}{I(2I-1)J_1(2J_1-1)}$$
(5.14)

$$\mathcal{U}_n = \frac{A'\frac{C}{2} + \frac{B'}{4} [\frac{3}{2}C(C+1) - 2I(I+1)J_2(J_2+1)]}{I(2I-1)J_2(2J_2-1)}$$
(5.15)

where

$$C = \frac{F_{max}(F_{max}+1) - J_i(J_i+1) - I(I+1)}{2}$$

$$i = 1,2$$
(5.16)

The parameters A,A',B and B' correspond to the hyperfine A,B coefficients, with the prime symbol denoting the excited state. Note that both (5.14) & (5.15) are exactly analogous to equation (2.16). Starting values for both are taken from the **parameters.dat** first guess values. The A,B coefficients, the parameter C and equations (5.14) and (5.15) are all in MHz, the unit that will be used throughout the computation and eventual fitting.

The transition energy matrix \mathcal{E}_{mn} is then declared, of identical dimension to \mathcal{T}_{mn} and its elements are defined as:

$$\mathcal{E}_{mn} = \mathcal{U}_n - \mathcal{L}_m \tag{5.17}$$

With both m-by-n matrices computed, a complete theoretical description of the HFS is now at hand. Both are printed to the file HFSdata.dat in the main folder for inspection if desired.

5.7 Spectrum Fitting and Parameter Extraction

From here, the final step in the analysis begins. HInSane selects, based on user input, one of the n integration files to fit the hyperfine spectrum. For information on HInSane operating procedures, see Appendix C.

A Root function is declared, containing as many peaks as there are allowed transitions in \mathcal{T}_{mn} . The peaks are represented as Voigt profiles, denoted $V(\nu)$, as detailed in equation (2.22). Both Gaussian and Lorentzian functions feature repeating parameters, which are forced to be identical for both: The peak standard deviation σ_{ν} and the mean ν_0 are forced to be identical, in addition to the normalisation constant A_0 . Thus, the individual peaks initially possesses a total of 4 fit parameters each.

A composite function is declared in Root, consisting of the linear addition of all peaks declared in the HFS simulation, in addition to a zeroth order background parameter:

$$\mathcal{F}(\nu) = c_0 + \sum_{i=1}^{n} V_i(\nu)$$
(5.18)

where c_0 is the background term and i indexes the peaks within the scan, with the summation running over the *n* peaks in scan range. Values form \mathcal{T}_{mn} determine the initial height (intensity) of the peaks, while the elements of \mathcal{E}_{mn} are ascribed to their respective means ν_0 . All other fit parameters are read from parameters.dat.

Performing spectrum fits using the variables ν_0 given by the HF simulation would, however, not return the hyperfine A,B coefficients, which represent the standard reported HFS quantification parameters.

To directly extract these from the fitting, equations (2.23) and (2.24) undergo another substitution, where the mean of each peak ν_0 is tied to the hyperfine A,B coefficients via:

$$\nu = \nu_{off} + (A'C' + B'D') - (AC - BD) + \delta_{IS}$$
(5.19)

$$D = \frac{3C(C+1) - 4I(I+1)J(J+1)}{8IJ(2I-1)(2J-1)}$$
(5.20)

where prime denotes the excited and unprimed refers to ground state in the

electronic scheme. ν_{off} represents an offset parameter, intended to compensate for beam energy uncertainty, generally corresponding to less then 10 volts in what is typically a total beam energy of 20KV, resulting in a ~ 200 MHz frequency uncertainty. On the other hand, δ_{IS} represents the isotope shift, manifest as a change in the centroid (the weighted average) of the hyperfine peaks due to changes in the nuclear charge distribution.

In practice there is no *a priori* method to distinguish between ν_{off} and δ_{IS} , so they are bunched together into a single fit parameter on the spectrum, which acts as a global offset parameter on all of the peaks - Parameter 22 in Table 9. Deconvolution of the two requires posterior analysis to determine the uncertainty in the beamline energy.

The parameters C,D,C',D' represent the Clebsch-Gordan couplings of the particular electron orbital states, with C being taken from equation (5.16). For the C',D' computations, the I,J,F values of the upper state are used.

With these considerations in hand, the standard mode of operation is then to run HInSane with a set of guess parameters. These should be ballpark figures, within about 10 to 15% of the actual values, to avoid divergences in the minimisation algorithm, Root-MINUIT. The fit quality is judged based on the χ^2 per degree of freedom (DOF), defined as:

$$\frac{\chi^2}{DOF} = \sum_{i=1}^m \frac{(D_i - \mathcal{F}_i)^2}{\mathcal{F}_i \times DOF}$$
(5.21)

where \mathcal{F}_i is the value of the fit function, evaluated at the same abscissa as the data point, D_i , for m data points in a given set. *DOF* represents the degrees of freedom in the file, corresponding to the m data points, minus the total number of fit parameters.



Figure 34: Absolute χ^2 per DOF residual versus integration bounds, in integer timebins. In the above example, the fifth entry (freqintegral5.dat) has the lowest residual χ^2 per DOF and is thus used to fit the hyperfine spectrum of 23 Na.

The optimal fit is extracted by successively integrating and fitting equation (5.18) to the HF spectra from $\frac{1}{n}$ of the EGH bounds to their full value, where n is the desired number of integration steps.

A plot of χ^2 obtained using files freqintegral1.dat to freqintegral20.dat is shown in Figure 34 for ²³Na. This is always saved to file as Chi2.dat, in the main folder. Further, the χ^2 per DOF, the A,B values and all peak information are stored in the file FitParameters.dat, located in the same directory.

HInSane automatically selects the integration file which returns a $\frac{\chi^2}{DOF}$ closest to unity for spectrum fitting and returns the associated fit parameters. The chi-square result is the only output parameter that the user must verify to gauge fit quality. Poor values indicate that a change of bounds or perhaps initial guess A,B parameters is in order.

All fit parameters returned by the Root spectrum fitting are shown in Table

Parameter	Units		
r	Ø		
σ	MHz		
А	MHz		
A'	MHz		
В	MHz		
B'	MHz		
Background	photon counts		
Peak Heights	photon counts		
$ u_0$	MHz		
SNR	Ø		

Table 10: List of fit parameters returned by HInSane, saved in FitParameters. Note that both Peak Heights and ν_0 are given for each individual peak.

10. These are saved to the file FitParameters.dat, located in the main folder. The former also contains information regarding user selected fit options, type of function used and nuclear spin.

Figure 35 shows the simulated HFS, the experimental data and the fit result, taking the fifth of twenty integration files, integrating over $\frac{5}{20}$ of the asymmetric EGH bounds on the timebunch.

The EGH bounds in Figure 35 were set to 1.5σ to the left and 3.5σ to the right of the EGH mean. Note that the initial guess width of the Voigts has been purposely underestimated to show the structure of the HF peaks.



Figure 35: Simulated, experimental and fit hyperfine spectrum of 23 Na, obtained by laser spectroscopy group data, integrated by HInSane (file 5 of 20). Note the thermal Doppler broadening on the experimental data renders the hyperfine peak structures unresolvable.

Par.	Value	Fit	Literature
A $[MHz]$	800	883.17(3.8)	$885.813\ 064\ 4(5)$
A' $[MHz]$	16.834	18.584(0.081)	18.534(15)
B'[MHz]	2.5	-7(14)	2.724(30)

Table 11: Comparison of input, returned and literature values for the 23 Na A,B coefficients. Note that A' is entered into parameters.dat as the ratio of A/A', as shown. The input value for A' works out to 16.8342 MHz. Literature values were obtained from [33]

Table 11 shows comparisons between the A,B coefficients and the accepted literature values. The fit $\frac{\chi^2}{DOF}$ was of 1.01871.

The fit performed by HinSane started with a value for the A coefficient which was about 10% off the literature value, The performance of the fit for the B' coefficient was relatively poor, with an uncertainty exceeding the fit value in magnitude. This result may be understood by inspection of equation (2.16): Considering the relative value of both the A and B coefficients, with the latter outweighing B by a factor of over 325, the sensitivity of the B coefficient is extremely small. The fitted A coefficient lies within 2.643 MHz (0.3%) of the accepted value, which is approximately equal to the B' coefficient value itself.

6 Conclusion & Outlook

The pioneering work of Thibault *et al.* at ISOLDE, which to this day remains authoritative for the rubidium isotope chain, was presented and discussed. The laser spectroscopy group at TRIUMF has, since 2010, undertaken a study of the extreme outlying rubidium isotopes, which were below detection thresholds for the ISOLDE group. Proton bombardment of a niobium target at TRIUMF was able to produce in excess of 10^4 ions/s for the neutron deficient $^{74-76}$ Rb, in addition to 78,78m Rb, which were all fluoresced in late 2010.

The hyperfine A,B coefficients, in addition to the measured MSCR values were successfully extracted for the aforementioned isotopes. This represented the first ever measurement of ⁷⁴Rb's charge radius which, given the former's involvement in superallowed beta decay, has ramifications from nuclear structure (⁷⁴Rb is at the drip line) to the unitarity of the CKM matrix [16]. In addition, the first spin assignment for ⁷⁵Rb was performed through the analysis of its hyperfine spectrum.

On the neutron rich side, after switching to a uranium carbide target, isotopes $^{92,98-100}$ Rb were produced, with yields again exceeding 10^4 ions/s, well above the detection threshold of the TRIUMF spectroscopy apparatus. While 92 Rb was fluoresced with relative ease, it was not possible to observe 98 Rb. The 92 Rb observations nevertheless represented the first time the isotope was sent into the RFQ cooler-buncher and fluoresced at TRIUMF. This was accomplished with relative ease, with run durations on the order of 10 minutes required to obtain a signal to noise ratio of more than 10. The isotope will be used as a frequency standard for further neutron deficient runs down the road. In addition to these developments, the spectroscopy group has overhauled their

data acquisition system, opting to use an MCS-based DAQ, allowing for greater flexibility and ease of operation. The author of this thesis was involved in the development of data analysis software, dubbed HInSane, which manipulates the new output data format to perform signal to noise reduction and hyperfine spectrum simulations and fits, based on user input parameters.

This data processing system, having been calibrated on the hyperfine spectrum of 23 Na, acquired at TRIUMF in late 2010, has been used in this thesis to perform 92 Rb fits with relative ease. The same program is currently being used by other members of the group to analyse spectra of francium isotopes, which are also being studied. It is the hope of the author that HInSane will be of continuing use to the group in the future. To this end, the programming aimed to allow adaptability and reusability, with sufficient commenting to avoid headaches should anyone attempt future modifications.

Appendix A: Neutron Deficient

Rubidium Spectra



Figure 36: Hyperfine spectra of $^{74-76,78,78m}$ Rb, collected at TRIUMF in late 2010. Note the fit functions are overlayed on the raw data. See Table 4, Section 3 for fit parameters.

Appendix B: MIDAS Data Bank Example

A typical MIDAS data bank, taken form the raw .mid file is shown in Figure 37. Note that two common events id's (Evid's) are shown: While Evid 5 corresponds to the raw PMT events (again in hex format), event ID 3 corresponds to a readback of other MCS board outputs, which for most experiments are left unoccupied. In principle, it would be possible to read in additional information, with up to 4 free MCS ports on the current board.

In a terminal environment, the mdump command may be used to display raw outputs. The standard terminal command will thus be:

mdump -f a -x run00354.mid

where the flag f (format) with option a produces ascii output. Doing so will produce a complete MIDAS dump to terminal, which will result in a sizeable output. Using this mode, the output should be piped to file using standard terminal syntax. Otherwise, to inspect a finite amount of data banks, the output flag -1 (length) may be used, followed by an integer specification of the desired bank output count.

Note that in online mode, during MCS operation, the mdump command will produce real time output dumping.

Event# 229 Evid:0003- Mask:0008- Serial:164- Time:0x4dbecfc0- Dsize:228/0xe4 #banks:5 - Bank list:-MCSUMCUMDBUGCYCLTHRC-Bank:MCSU Length: 16(I*1)/4(I*4)/4(Type) Type:Real*4 (FMT machine dependent) $1 - 6.540 + 02 \ 0.000 + 00 \ 0.000 + 00 \ 0.000 + 00$ Bank:MCUM Length: 16(I*1)/4(I*4)/4(Type) Type:Real*4 (FMT machine dependent) 1-3.145e+03 2.000e+00 1.000e+00 0.000e+00 Bank:DBUG Length: 48(I*1)/12(I*4)/12(Type) Type:Real*4 (FMT machine dependent) 1-0.000e+00 1.000e+02 1.000e+02 1.000e+02 1.000e+02 0.000e+00 0.000e+00 0.000e+00 9-0.000e+00 0.000e+00 0.000e+00 0.000e+00 Bank:CYCL Length: 36(I*1)/9(I*4)/9(Type) Type:Real*4 (FMT machine dependent) $1 - 1.000e + 00 \ 1.650e + 02 \ 3.400e + 01 \ 0.000e + 00 \ 1.000e + 00 \ 1.000e + 00 \ 1.660e + 02 \ 3.400e + 01 \ 0.000e + 00 \ 1.000e + 00 \ 0.000e + 0$ 9-9.300e-01 Bank:THRC Length: 36(I*1)/9(I*4)/9(Type) Type:Unsigned Integer*4 0x00000000 9-0x00000000 Event# 230 Evid:0005- Mask:0020- Serial:32- Time:0x4dbecfc1- Dsize:1692/0x69c #banks:5 - Bank list:-HISIHIS0HIS1HIS2HIS3-Bank:HISI Length: 24(I*1)/6(I*4)/6(Type) Type:Real*4 (FMT machine dependent) 1-1.650e+02 5.000e+00 9.200e-01 -8.664e-03 3.200e+01 5.000e+00 Bank:HIS0 Length: 400(I*1)/100(I*4)/100(Type) Type:Unsigned Integer*4 1- 0x0000029e 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 9- 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 17- 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 25- 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 33- 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 41- 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 49- 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 57- 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 65- 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 73- 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019

81- 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 89- 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019 0x00000019

97- 0x00000019 0x00000019 0x00000019 0x00000019

Figure 37: The raw midas file output. Bank labels HIS0-HIS3 correspond to four separate MCS inputs, of which only HIS0 (PMT output) is used. MCSU corresponds to a bank of 4 supplemental (unused) inputs, while MCUM represents the overall integral of the former. DBUG (debug) currently serves no purpose, while CYCL contains current and overall cycle information. THRC is unused.

Appendix C: HInSane

Standard Operating Procedure

While HInSane is designed to facilitate hyperfine spectrum parameter extraction, it nevertheless requires the user's judgement to maximise fit quality. A brief operational summary is thus given.

The very first step is to ensure **parameters.dat** is properly filled out. Particular attention should be given to the following parameters, which are involved in the channel to energy conversion:

- Isotope Mass
- V_{RFQ}
- Transition Wavenumber
- Laser Wavenumber

It is recommended to use as many available significant digits as available for the input values, as they determine the final values of the x-axis in the spectrum fitting, as can be seen in equation (2.25). All numbers are to be in decimals, as fractions cannot be read.

With the energy parameters now taken care of, the next step should be to run HInsane with preliminary guess A,B coefficients. HInSane is executed in a standard unix terminal environment by typing, for example:

HInSane run00354.mid

Where the previous command would use the file run00354.mid to produce the output. Once this command has been entered, HInSane requires no further

input and will cycle through its subroutines until complete. The program's sequence of operation is as follows:

- 1. Declaration of Root histograms
- 2. Linear fitting of Kepco+Harrison voltage to channel function
- 3. Reading of parameters.dat
- 4. Timebunch fittings (Gaussian & EGH)
- 5. Computation & declaration of simulated HFS
- 6. Determination of scan range
- 7. Determination of peak count within scan range
- 8. Fitting of integral files and determination of best SNR
- 9. Re-fitting of best SNR integral and final output to files

The first run of the program will probably not produce the best final output result. Rather, it will serve as a benchmark for further fitting. Immediately after the timebunch fittings, HInSane outputs to console information regarding the scan range and peak positions. The following sample is taken from the file run00580.mid, consisting of ²⁰⁸Fr:

Declaring predicted HFS peaks. ROOT histogram declared by determining the frequency domain scanned by the Kepco and Harrison sweep.

In order for a peak to be included in the fit routine, it is necessary that the simulated peak be found within the range covered by the scan, otherwise the peak is excluded.

Note that the mean of each HFS peak WILL be influenced by the parameters.dat input parameters. If no peaks fall within scan range, consider tweaking the inputs

Note: All frequencies are relative to D2 centroid
Hint: if fitting fails, add MHz value of peak in middle of
spectrum with scan midpoint as isotope shift. Kepco+Harrison
sweep bounds in MHz - From 23803.7105 to
27722.5748 Scan midpoint (MHZ): 25763.1426

With the first run complete, one now has in hand both the scan range and a Root printout of the PMT count spectrum. The above example thus runs from 23803 to 27722 MHz from the D_2 line of 208 Fr.

The next step is to determine the location of the hyperfine peaks - This will aid in the determination of the A,B coefficients. The output .root file containing the integrated DAQ spectrum is located in the file /root/HFSpeaks.root, under the item DAQ_Spectrum.

It is then up to the user to identify the approximate position of the hyperfine peaks in the data set. The determination may be accurate to around 100MHz. The location of the peaks will aid in the next step of the fitting routine: Finding optimal first guess A,B coefficients.

With the peak locations noted, one should proceed to vary the A,B coefficients in parameters.dat and looking at the output peak positions returned by HIn-Sane in the console output, immediately following the scan range indication:

Note: All frequencies are relative to D2 centroid
Hint: if fitting fails, add MHz value of peak in middle of
spectrum with scan midpoint as isotope shift. Kepco+Harrison
sweep bounds in MHz - From 23803.7105231285 to
27722.5748766661 Scan midpoint (MHZ): 25763.1426998973

Mean: 24430.5058 leftbound: 23803.7105 rightbound: 27722.5748 Peak (no IS): 1 centroid (no IS): 26097.5058 with IS: 24430.5058 Mean: 24913.2216 leftbound: 23803.7105 rightbound: 27722.5748 Peak (no IS): 2 centroid (no IS): 26580.2216 with IS: 24913.2216 Mean: 25464.2493 leftbound: 23803.7105 rightbound: 27722.5748
Peak (no IS): 3 centroid (no IS): 27131.2493 with IS: 25464.2493 Mean: -24454.7783 leftbound: 23803.7105 rightbound: 27722.5748 Peak 4 centroid (no IS): -22787.7783 with IS: -24454.7783 - NOT IN SCAN RANGE Mean: -23903.7506 leftbound: 23803.7105 rightbound: 27722.5748 Peak 5 centroid (no IS): -22236.7506 with IS: -23903.7506 - NOT IN SCAN RANGE Mean: -23307.7861 leftbound: 23803.71052 rightbound: 27722.5748 Peak 6 centroid (no IS): -21640.7861 with IS: -23307.7861 - NOT IN SCAN RANGE

Changing the A,B coefficients will change the spacing between HF peaks. It is then necessary to adjust the isotope shift in parameters.dat to offset the change in overall frequency brought forth by a change in A,B's. Once spacing between peaks, as well as the frequency mean (centroid) of each peak in scan range is sufficiently close to the experimental data in DAQ_Spectrum (close to about 100MHz), HInSane should be able to perform an optimal fit, returning the optimal χ^2 per DOF for the given spectrum.

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